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Dissipation and dilatation

Dissipation and dilatation rates in premixed turbulent flames

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Velocity dilatation, as well as total, solenoidal, and dilatational dissipation rates of the total flow kinetic energy are extracted from three different direct numerical simulation databases obtained by three independent research groups using different numerical codes and methods (e.g., single-step chemistry and complex chemistry flames) from six different premixed turbulent flames associated with flamelet, thin reaction zone, and broken reaction zone regimes of turbulent burning. Results show that dilatational dissipation can be larger than solenoidal dissipation in the flamelet regime and is substantial in the thin reaction zone regime. Accordingly, the influence of combustion-induced thermal expansion on dissipation rate is not reduced to an increase in the mixture viscosity by the temperature. A simple criterion for identifying conditions associated with significant dilatational dissipation is discussed and dilatational dissipation due to the influence of turbulence on mixing in preheat zones is argued to play a role even at high Karlovitz numbers Ka . In particular, the magnitude of dilatation fluctuations and probability of finding negative local dilatation are increased by Ka , thus, implying that the impact of molecular transport of species and heat on the dilatation increases with increasing Karlovitz number.

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I. INTRODUCTION

The mean rate $\overline{\rho\epsilon}$ of viscous dissipation of kinetic energy of a turbulent flow (or dissipation rate for brevity) is one of the most important quantities in the turbulence theory.¹⁻⁶ The dissipation rate is defined as follows:

$$\overline{\rho\epsilon} \equiv \overline{\tau_{ij}S_{ij}}, \quad (1)$$

where

$$\tau_{ij} = 2\mu \left(S_{ij} - \frac{1}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k} \right) + \mu_v\delta_{ij}\frac{\partial u_k}{\partial x_k} \quad (2)$$

is the viscous stress tensor, $S_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2$ is the strain rate tensor, μ is the dynamic viscosity, μ_v is the bulk viscosity, u_i is the i -th component of the velocity vector \mathbf{u} , and δ_{ij} is the Kronecker delta, with the summation convention applying to repeated indexes. If $\mu_v = 0$, the dissipation rate can be decomposed as follows:⁷⁻¹¹

$$\overline{\rho\epsilon} = \overline{\mu\omega^2} + \frac{4}{3}\overline{\mu\Theta^2} + 2\overline{\mu\frac{\partial^2}{\partial x_i\partial x_j}(u_iu_j)} - 4\overline{\mu\frac{\partial}{\partial x_i}(u_i\Theta)}, \quad (3)$$

where $\omega^2 = \omega_k\omega_k$ is the enstrophy, $\omega_i = \epsilon_{ijk}\partial u_j/\partial x_k$ is the i -th component of the vorticity vector, $\Theta = \partial u_k/\partial x_k$ designates dilatation, and ϵ_{ijk} is the cyclic permutation tensor. The first and second terms on the right hand side (RHS) of Eq. (3) are known as solenoidal and dilatational dissipation,⁷ respectively, whereas the third and fourth terms are mixed terms, i.e. they contain contributions from both solenoidal and dilatational velocity components. In the following, these two mixed terms will be considered jointly. If the viscosity μ is constant, the mixed terms asymptotically vanish at high Reynolds numbers because they contain spatial derivatives of mean quantities, whereas the solenoidal and dilatational dissipations involve mean values of squares of local spatial derivatives. For the same reason, dissipation rates evaluated using total or fluctuating velocity fields are asymptotically equal to one another at high Reynolds numbers.

In incompressible turbulent flows, dilatation vanishes and the dissipation rate is asymptotically equal to the solenoidal dissipation at high Reynolds numbers. If density varies due to pressure variations in high-speed flows, heat release at almost constant pressure in low-speed reacting flows, or both pressure variations and heat release (e.g., combustion in supersonic flows), dilatational dissipation plays a role. For instance, in high-speed non-reacting flows, a ratio

$$\chi = \frac{4}{3}\frac{\overline{\Theta^2}}{\overline{\omega^2}} \quad (4)$$

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of dilatational and solenoidal dissipations was reported^{7,12} to scale as αM_t^2 in a first approximation, with the factor α being substantially less than unity. Here, $M_t = u'/C$ is the turbulence Mach number, u' is the root-mean-square (rms) velocity, and C is a representative speed of sound. In subsequent studies of compressibility effects on turbulence characteristics (spectra, a ratio of dilatational kinetic energy to solenoidal kinetic energy, a ratio of dilatational dissipation to solenoidal dissipation, etc.) in homogeneous non-reacting flows,^{13–18} dependence of the ratio χ on M_t was clarified, e.g. $\chi \propto M_t^4$ at $M_t < 0.4$,¹⁶ with substantial dependence of χ on the turbulent Reynolds number $Re_\lambda = u'\lambda/\nu$ being also documented, as reviewed elsewhere.¹⁷ Here, λ is the Taylor length scale and $\nu = \mu/\rho$ is the kinematic viscosity of the fluid.

Recently, Donzis and John¹⁷ have analyzed a large set of published and their own direct numerical simulation (DNS) data and have shown that the ratio χ is proportional to a ratio of dilatational and solenoidal turbulent kinetic energies, k_d/k_s , and k_s , respectively, with these two ratios varying by almost ten and five orders of magnitude, respectively. When the same data are plotted vs. M_t , the scatter of the data is significantly more pronounced. More specifically, at $M_t < 0.2$, DNS data generated by Donzis and John¹⁷ using either solenoidal or dilatational forcing differ drastically from one another, i.e., the ratio χ can be as large as 10^3 in the latter case, whereas $\chi \ll 1$ in the former case (if $M_t < 0.2$). An important role played by the ratio of k_d/k_s was also revealed in a recent study of compressibility effects in mixing of passive scalars in homogeneous flows.¹⁸

In subsonic reacting flows, non-negligible values of the ratio χ were found in non-premixed flames with homogeneous initial conditions at $0 < Ma_t < 0.5$ ^{19–22} and in a spatially developing shear layer at $Ma_t \ll 1$.²³ In all these studies, χ was significantly less than unity. Recently, Teng et al.¹⁶ numerically explored evolution of initially unmixed reacting flows embedded into homogeneous isotropic turbulence. The obtained DNS data show that the ratio χ depends substantially on a heat release parameter (a ratio of the heat of reaction to a reference enthalpy in the cited paper) and a Damköhler number Da , which characterizes a ratio of the turbulence reaction time scales, whereas the dependence of χ on Re_λ is weakly pronounced at high Da . Under conditions of the discussed DNS, the ratio χ can be larger than unity if $M_t = 0.6$ and the Damköhler number is as large as 3000. However, the computed χ is significantly less than unity for $M_t = 0.2$ even if $Da = 3000$.

Accordingly, to the leading order, the influence of reaction-induced density variations on the dissipation rate may be assumed to be controlled by an increase in the solenoidal dissipation due to an increase in the viscosity with the temperature in reacting flows characterized by a low Mach number.^{16,20–22} Contrary to the aforementioned studies of the influence of heat release on dissipation rate in the non-premixed mode of turbulent burning, the present authors are not aware of evaluation of the ratio χ in premixed flames (note that such a flame is characterized by significant spatial gradient of the mean flow velocity in the direction normal to the mean flame surface). Nevertheless, in a recent DNS study^{24,25} of highly turbulent

premixed flames, the influence of combustion-induced thermal expansion on small-scale turbulence was also attributed to the increase in the mixture viscosity.

Based on the recent findings by Donzis and John,¹⁷ John et al.,¹⁸ and Teng et al.,¹⁶ one may hypothesize that, in premixed turbulent flames characterized by $M_t \ll 1$, the ratio χ depends on Re_λ , k_d/k_s , the density ratio $\sigma = \rho_u/\rho_b$, and Da (note that the Karlovitz number defined later is proportional to Re_λ/Da in premixed flames). In other words, if $M_t \ll 1$,

$$\chi = f(Re_\lambda, k_d/k_s, \sigma, Da), \quad (5)$$

where f is a “universal” non-dimensional function. To our knowledge, there are neither theories nor numerical data on the dependence of the ratio χ on the aforementioned non-dimensional parameters. On the contrary, as reviewed elsewhere,^{26,27} numerical modeling of premixed turbulent combustion relies commonly on theories and models of constant-density turbulence characterized by $\nabla \cdot \mathbf{u} = 0$ and vanishing dilatational dissipation. Since dissipation rate plays a key role in the turbulence theory,^{1–6} eventual change of the physical nature of dissipation in premixed flames when compared to constant-density turbulence, i.e. appearance of dilatational dissipation in the former case, requires thorough investigation and, in particular, evaluation of the ratio χ in the case of premixed turbulent burning.

Accordingly, the major goals of the present study are (i) to examine dilatation in premixed turbulent flames characterized by a very low Mach number and various (small, moderate, and high) Karlovitz numbers and (ii) to demonstrate that dilatational dissipation can play a substantial role in such flames. For this purpose, three DNS databases that are described briefly in the next section were analyzed. Results are reported and discussed in the third section, followed by conclusions.

II. DNS ATTRIBUTES

Analyzed in the present work are the following three DNS databases: (i) Nagoya data that were created by Nishiki et al.^{28,29} about 20 years ago and were subsequently explored by various research groups,^{30–34} (ii) Bangalore data that were computed recently by Dave and Chaudhuri⁵⁵ and were subsequently analyzed by two of the present authors,^{56,57} and (iii) KAUST data^{58–60} that were also used by various research groups.^{61–64} In the following, major attributes of these three DNS series are briefly summarized. The reader interested in more details is referred to the cited papers.

All these unsteady three-dimensional simulations had certain common features. First, they addressed statistically planar and one-dimensional, adiabatic premixed flames propagating in rectangular channels. Second, the governing equations were solved in compressible form. Third, homogeneous isotropic turbulence was generated in a separate box, was injected into the computational domain through the left boundary $x = 0$ and decayed along the direction x of the mean flow. Fourth, the simulated flows were periodic in y and z directions. Fifth, a planar laminar flame was embedded into tur-

bulent flow in the computational domain at $t = 0$. Subsequently, the mean inflow velocity was changed twice^{28,29} or gradually^{55,58–60} to match turbulent flame speed. Sixth, in the present paper, the combustion progress variable is defined as follows

$$c = \frac{T - T_u}{T_b - T_u}, \quad (6)$$

where T is the temperature and subscripts u and b designate unburned reactants and burned products, respectively.

Major characteristics of the simulated flames are reported in Table I. Here, S_L and $\delta_L = (T_b - T_u) / \max |\nabla T|$ are the laminar flame speed and thickness, respectively, $\sigma = \rho_u / \rho_b$ is the density ratio, u' and L are the rms velocity and an integral length scale, respectively, of turbulence generated in a box, $\tau_t = L / u'$ is the eddy-turn-over time, $Re_t = u' L / \nu_u$ is the turbulent Reynolds number, $Ka = (u' / S_L)^2 Re_t^{-1/2} (S_L \delta_L / \nu_u)$ is the Karlovitz number, and ν_u is the kinematic viscosity of unburned mixture. The Karlovitz number is proportional to a ratio of the flame time scale $\tau_f = \delta_L / S_L$ to the Kolmogorov time scale $\tau_K = (\nu_u / \bar{\epsilon})^{1/2}$, with the coefficient of proportionality $\sqrt{C_d}$ being of unity order if $\bar{\epsilon} = C_d u'^3 / L$.^{2,5} Certain specific features of the discussed DNS databases are noted in the following subsections.

A. Nagoya DNS database

A computational domain of $8 \times 4 \times 4$ mm was resolved using a uniform rectangular ($2\Delta x = \Delta y = \Delta z$) mesh of $512 \times 128 \times 128$ points.

Combustion chemistry was reduced to a single reaction, the Lewis and Prandtl numbers were equal to 1.0 and 0.7, respectively, and the mixture state was completely characterized with a single combustion progress variable c . Temperature dependence of molecular transport coefficients was taken into account, e.g., $\nu = \nu_u (T / T_u)^{1.7}$.

Flames H and L are characterized by high and low density ratios, respectively, with all other parameters being approximately equal (the first and second lines, respectively, in Table I). These flames are well associated with the flamelet combustion regime,⁶⁵ as shown elsewhere.³⁷

Results reported in the following were averaged over transverse planes and a time interval of $1.5\tau_t$, associated with fully developed flames, as discussed in detail elsewhere.⁵¹

B. Bangalore DNS database

The DNS data were computed adopting the Pencil code.⁶⁶ A computational domain of $19.18 \times 4.8 \times 4.8$ mm was discretized using a uniform mesh of $960 \times 240 \times 240$ nodes.

A lean (the equivalence ratio $\Phi = 0.81$) and slightly preheated ($T_u = 310$ K) hydrogen-air flame was studied using detailed reaction mechanism (9 species, 21 reactions) by Li et al.⁶⁷ and mixture-averaged transport coefficients, which depended on temperature. The simulation conditions (flame IIS-70

FIG. 1. Dissipation rate normalized using $\mu_u S_L^2 / \delta_L^2$ and various contributions to it vs. Reynolds-averaged combustion progress variable \bar{c} . (a) Nagoya flame H, (b) Nagoya flame L, (c) Bangalore flame IIS, (d) KAUST flame A, (e) KAUST flame B, (f) KAUST flame C.

in the third line in Table I, where IIS is an abbreviation of Indian Institute of Science) are associated with the thin reaction zone regime⁶⁵ of turbulent burning.

As discussed in detail elsewhere,^{56,57} results reported in the following were averaged over transverse planes and various instants (54 snapshots stored each $5 \mu s$ over the time period $1.401 \text{ ms} \leq t \leq 1.566 \text{ ms}$).

C. KAUST DNS database

In cases A and B, a computational domain of $20 \times 10 \times 10$ mm was discretized using a uniform mesh of $512 \times 256 \times 256$ nodes, whereas in case C, a computational domain of $8.32 \times 2.08 \times 2.08$ mm was discretized using a uniform mesh of $1280 \times 320 \times 320$ nodes. To solve the governing equations, an eighth-order central difference and an explicit fourth-order Runge-Kutta schemes were employed.⁵⁸

A lean ($\Phi = 0.70$) hydrogen-air flame ($T_u = 300$ K) was studied using a detailed reaction mechanism (9 species, 19 reactions) by Burke et al.⁶⁸ and mixture-averaged transport coefficients, which depended on temperature. The simulation conditions (the three bottom lines in Table I) are associated with flamelet, thin reaction zone, and broken reaction zone regimes⁶⁵ of turbulent burning in cases A, B, and C, respectively.

As discussed in detail elsewhere,⁶³ results reported in the following were averaged over transverse planes and six different instants in each case, i.e., at $t/\tau_t = 0.57, 0.67, 0.77, 0.86, 0.96$, and 1.05 in case A and at $t/\tau_t = 4.1, 4.8, 5.5, 6.2, 6.8$, and 7.5 in cases B and C.

Since the major characteristics of the Nagoya flame H and the KAUST flame A are similar and both flames are associated with flamelet combustion regime, comparison of results computed in these two cases allows us to examine the influence of combustion chemistry and diffusive-thermal effects^{69–71} on the dissipation rate. Comparison of results obtained from the Bangalore flame IIS and the KAUST flame B, which both have similar major characteristics and are associated with thin reaction zone regime of turbulent burning, allows us to check the consistency of the two databases. Moreover, comparison of results obtained from the KAUST flames A, B, and C allows us to explore the influence of Karlovitz number on the relation between the dilatational and solenoidal dissipations.

TABLE I. Characteristic parameters of DNS cases

Flame	S_L , m/s	δ_L , mm	σ	u' , m/s	L , mm	τ_t , ms	Re_t	Ka	$Ka/(\sigma - 1)$	M_t
H	0.6	0.217	7.53	0.53	3.5	6.6	96	0.60	0.09	0.0015
L	0.416	0.158	2.50	0.53	3.5	6.6	96	0.64	0.43	0.0015
IIS	1.84	0.36	6.15	6.7	3.1	0.46	950	19.0	3.7	0.02
A	1.36	0.36	5.95	0.95	5.0	5.3	227	0.75	0.15	0.002
B	1.36	0.36	5.95	6.8	5.0	0.74	1623	14.4	2.91	0.02
C	1.36	0.36	5.95	19.0	1.4	0.076	1298	126	25.5	0.055

III. RESULTS AND DISCUSSION

A. Comparison of solenoidal and dilatational dissipations

Figure 1 shows the total (solid lines), solenoidal (dashed lines), and dilatational (dotted-dashed lines) dissipations extracted from the six DNS data sets, as well as the sum (double-dashed-dotted lines) of the last two terms on the RHS of Eq. (3), referred to as “mixed.” The following trends are worth noting.

First, in all six cases the sum of the last two terms on the RHS of Eq. (3), whether it is positive or negative, is significantly less than the total dissipation, including flames H and L for which the turbulent Reynolds number is rather small (Figs. 1a and 1b).

Second, for flames H, L, and A in the flamelet combustion regime, the dilatational dissipation can be larger than the solenoidal dissipation. In flame H, characterized by a low Ka and a high density ratio, the ratio χ defined by Eq. (4) is significantly larger than unity in the entire flame brush, with the exception of its trailing zone ($\bar{c} > 0.95$). In flame L, characterized by a comparable Ka , but a significantly lower density ratio, the ratio χ is smaller (larger) than unity at $\bar{c} < 0.4$ ($\bar{c} > 0.4$, respectively). This trend is attributed to decay of the turbulence in the direction of the mean flow and a weak (due to a low density ratio) influence of baroclinic torque on vorticity within the L flame brush.³⁶ In flame H, such an influence is much stronger, as discussed in detail elsewhere.^{36,343} In flame A characterized by a slightly higher (when compared to flame H) Ka and a lower density ratio, the ratio χ is smaller (larger) than unity at $\bar{c} > 0.4$ ($\bar{c} < 0.4$, respectively). Differences in the behaviour of the ratio χ in flame A compared to flames H/L stem not only from complex-chemistry³⁴⁶ but also from diffusive-thermal effects, i.e. significant local³⁴⁷ variations in the temperature and equivalence ratio due to imbalance of heat and species fluxes from and to reaction zones³⁴⁸ curved and strained by turbulent eddies. Such effects are well³⁴⁹ known to play an important role in lean hydrogen-air turbulent³⁵⁰ flames, as reviewed elsewhere,^{69–71} and, in particular, can significantly³⁵¹ reduce local burning rate and combustion temperature³⁵² in negatively curved reaction zones. Since the probability³⁵³ of finding such reaction zones is higher at large \bar{c} due to³⁵⁴ purely topological reasoning, diffusive-thermal effects could³⁵⁵ substantially reduce dilatational dissipation at large \bar{c} in lean³⁵⁶ hydrogen-air turbulent flames.³⁵⁷

Third, even in flames IIS and B, characterized by $Ka > 10$ ³⁵⁸ and associated with the thin reaction zone regime of premixed³⁵⁹

burning, differences between the total and solenoidal dissipations are significant, implying that the dilatational dissipation is not negligible.

Fourth, in flame C, characterized by $Ka > 100$ and associated with the broken reaction zone regime of premixed turbulent burning, the total dissipation is mainly controlled by the solenoidal dissipation. This observation is consistent with recent DNS data that were also obtained from highly turbulent flames.^{24,25} Nevertheless, even in this case, dilatational dissipation is substantial at $\bar{c} < 0.1$. Physical mechanisms that could explain this observation will be discussed later. The rapid decrease in $\overline{\rho\epsilon}$ with \bar{c} observed in Fig. 1f is attributed to turbulence decay due to an increase in the mixture viscosity with increasing temperature.

All in all, Fig. 1 shows that (i) dilatational dissipation can play an important role even at low Mach numbers and (ii) in the flamelet and thin reaction zone regimes of premixed burning, the influence of combustion-induced thermal expansion on dissipation rate is not only due to an increase in the mixture viscosity by the temperature, as commonly believed. Rather, the combustion-induced thermal expansion changes the physical nature of the dissipation, shifting from the dissipation of vortices in constant-density turbulence to the dilatation-controlled dissipation in a premixed flame. Such a fundamental change in the nature of the dissipation in premixed flames casts doubts on the direct application of conventional constant-density turbulence models for simulations of premixed combustion. Other phenomena associated with the influence of combustion-induced thermal expansion on turbulence in premixed flames are reviewed elsewhere.^{26,27}

B. A simple criterion to estimate importance of dilatational dissipation

The simplest estimate of a criterion for indicating importance of dilatational dissipation can be obtained by comparing the magnitude of dilatation in the unperturbed laminar flame, i.e. $(\sigma - 1)S_L/\delta_L$, with the mean magnitude τ_K^{-1} of velocity gradients generated by the smallest eddies. Accordingly, dilatational dissipation is expected to play a minor role if $Ka/(\sigma - 1)$ is significantly larger than unity. As reported in Table I, these values are consistent with the results shown in Fig. 1f. A similar criterion of importance of thermal expansion effects in premixed turbulent flames was earlier proposed by Bilger,⁷² but based on a different reasoning. Recent DNS data by MacArt et al.^{73,74} are also consistent with such a cri-

360 terion, while dilatational and solenoidal dissipations are not
361 compared in the cited papers.

362 Nevertheless, the above simple criterion should be consid-
363 ered with a few cautions. First, it compares a statistically
364 averaged turbulence characteristic, i.e. τ_K^{-1} , with dilatation
365 $(\sigma - 1)S_L/\delta_L$ in the local laminar flame. To be more consis-
366 tent, multiplication of the dilatation with a probability γ of
367 finding such local flames should be used when comparing dil-
368 atational and solenoidal dissipations in a premixed turbulent
369 flame. Accordingly, $Ka/(\sigma - 1)$ should be compared with
370 $\gamma < 1$, rather than unity. Since the probability γ is likely to in-
371 crease with increasing Ka in moderately turbulent flames and
372 to reach a plateau close to unity at $Ka \gg 1$ and $Da \ll 1$,⁷⁵
373 the actual quantitative criterion is expected to be more com-
374 plicated.

375 Second, since combustion increases the mixture viscosity,
376 and hence τ_K , evaluation of this time scale at a temperature
377 higher than T_u , e.g. $(T_u + T_b)/2$, appears to be more consistent.
378 In such a case, $Ka/(\sigma - 1)$ should be compared with $\gamma[(1 +$
379 $\sigma)/2]^{0.85}$ if $v = v_u(T/T_u)^{1.7}$. For typical values of σ ,⁴¹²
380 the factor of $\gamma[(1 + \sigma)/2]^{0.85}$ could be sufficiently close to unity
381 in the vicinity of the boundary of the domain of importance of
382 dilatational dissipation, but further research into the discussed
383 criterion is definitely required.

384 Third, in premixed turbulent flames, dilatational dissipation
385 can result not only from heat release, but also from the in-
386 fluence of turbulence on molecular mixing in the local flame
387 zones characterized by a negligible heat release rate. To il-
388 lustrate such an effect in a simple manner, let us consider
389 the following low-Mach-number transport equation for the
390 temperature^{76,78}

$$391 \quad c_p \rho \frac{\partial T}{\partial t} + c_p \rho u_k \frac{\partial T}{\partial x_k} = c_p \frac{\partial}{\partial t} (\rho T) + c_p \frac{\partial}{\partial x_k} (\rho T u_k) \\ 392 \quad = - \frac{\partial J_{k,T}}{\partial x_k} + \dot{\omega}_T, \quad (7)$$

393 where c_p is the mixture heat capacity at constant pressure, $\dot{\omega}_T$
394 is the heat release rate, and the symbol $J_{k,T}$ designates the k -th
395 component of the flux vector J_T , which involves fluxes due to
396 molecular transport of heat and species. Using the ideal gas
397 state equation of $pW = \rho RT$ and considering the asymptotic
398 case of a low Mach number $M \ll 1$, which is typical for pre-
399 mixed flames,^{76,78} the product of ρT may be substituted with
400 $\rho T = \rho_u T_u [(W/W_u) + O(M^2)]$. Here, W is molecular weight
401 of the mixture and R is the universal gas constant. Accord-
402 ingly, Eq. (7) reads⁷⁸

$$403 \quad \Theta \equiv \frac{\partial u_k}{\partial x_k} = \frac{R}{c_p p_u} \left(- \frac{\partial J_{k,T}}{\partial x_k} + \dot{\omega}_T \right) \\ 404 \quad - \frac{1}{W_u} \left(\frac{\partial W}{\partial t} + u_k \frac{\partial W}{\partial x_k} \right). \quad (8)$$

405 Furthermore, variations in the molecular weight W are weak
406 in a typical premixed flame, where $W \approx W_u$ is controlled by
407 the molecular weight of N_2 to the leading order. Accord-
408 ingly, the ideal gas state equation is commonly simplified to
409 $\rho T = \rho_u T_u$ in the premixed combustion literature.⁷⁶⁻⁷⁸ In such

FIG. 2. Typical 2D images of heat release rate expressed in W/m^3 (top row), normalized dilatation rate $\Theta/[(\sigma - 1)S_L/\delta_L]$ (middle row), and normalized dilatational dissipation $4\mu\Theta^2/(3\mu_u S_L^2/\delta_L^2)$ (bottom row, with the color scale being logarithmic) in the KAUST flames A (left column), B (middle column), and C (right columns).

FIG. 3. Probability Density Functions $P(\Theta)$ for the local instantaneous dilatation $\Theta(x, t)$ normalized using $(\sigma - 1)S_L/\delta_L$ and conditioned to various values of the local instantaneous $c(x, t)$, specified in legends. (a) Bangalore flame IIS, (b) KAUST flame A, (c) KAUST flame B, (d) KAUST flame C.

a simplified case and if $J_T = -\rho \kappa c_p \nabla T$, Eq. (7) reads⁷⁹⁻⁸¹

$$\Theta = \frac{1}{\rho_u T_u c_p} \left[\frac{\partial}{\partial x_k} \left(\rho \kappa c_p \frac{\partial T}{\partial x_k} \right) + \dot{\omega}_T \right] \\ = \frac{\rho S_d}{\rho_u T_u} |\nabla T| = \frac{\rho(T_b - T_u)}{\rho_u T_u} S_d |\nabla c|, \quad (9)$$

where κ designates molecular heat diffusivity of the mixture and $S_d \equiv [\nabla \cdot (\rho \kappa c_p \nabla T) + \dot{\omega}_T]/(\rho c_p |\nabla T|)$ is a displacement speed⁷⁷ of the iso-surface $T(x, t) = \text{const}$.

Even if time and spatial derivatives of the pressure p and molecular weight W are neglected in Eq. (9), this simplified equation offers an opportunity to illustrate that the local dilatation may be significantly affected by molecular fluxes in preheat (and, to a lesser extent, in radical recombination) zones associated with low reaction rates. Moreover, molecular mixing in turbulent flows is known to be significantly affected by turbulent eddies.² Accordingly, at small and large $c(x, t)$, the local dilatation could be controlled by turbulence if it is sufficiently strong and the sign of Θ may be not only positive, but also negative (contrary to unperturbed laminar premixed flames where dilatation is always positive). Indeed, in Eq. (9), the dilatation Θ is proportional to the displacement speed S_d , with negative displacement speeds being well documented in DNS studies of highly turbulent premixed flames.^{55,82-87} Henceforth, dilatation that stems from the influence of turbulent eddies on molecular mixing in zones where the temperature field is non-uniform due to combustion is called turbulence-controlled dilatation for brevity. Since both this influence and the negative displacement speeds are more pronounced in more intense turbulence, that dilatation could play a substantial role even at a high Karlovitz number and, in particular, could notably affect the dissipation rate. Appearance of zones characterized by negative dilatation and substantial dilatational dissipation is observed upstream of the heat release zone in images plotted in Fig. 2 for the KAUST flames B and, especially C. Certain DNS data that are consistent with this hypothesis are presented in the next subsection.

C. Influence of Karlovitz number on dilatation

Figure 3 shows variations in the conditioned Probability Density Function (PDF) $P(\Theta^*)$ with the local instantaneous

FIG. 4. Correlation coefficients $C_{a,b} = (\overline{ab} - \bar{a}\bar{b})/(\overline{a^2} \overline{b^2})^{1/2}$ between dilatation and (a) combustion progress variable c , (b) strain rate a_t , (c) heat release rate $\dot{\omega}_T/c_p$, and (d) the magnitude $|\nabla c|$ of the gradient of the combustion progress variable vs. Reynolds-averaged combustion progress variable \bar{c} . Abbreviation IIS refers to flame simulated in the Indian Institute of Science.

combustion progress variable $c(x,t)$ that the PDF is conditioned to. These PDFs have been sampled from the entire computational domains in the complex-chemistry cases IIS, A, B, and C. Henceforth, the symbol Θ^* designates the local instantaneous dilatation rate $\Theta(x,t)$ normalized using $(\sigma - 1)S_L/\delta_L$. The following trends are worth noting.

First, the variations in $P(\Theta^*)$ with $c(x,t)$ are non-monotonic. That is, in the upstream region, as $c(x,t)$ increases from 0.1 to 0.3, the peak value of the normalized dilatation increases while the PDF distribution broadens (with an exception for case IIS). As $c(x,t)$ increases further from 0.3 to 0.7, the PDF distribution becomes narrower while the peak value decreases. This behavior is attributed to the fact that the dilatation and heat release rate peak in the interval $0.2 < c < 0.3$ in the unperturbed laminar flames associated with the Bangalore and KAUST simulations. Moreover, the monotonic attenuation in turbulence intensity leads to a narrower PDF distribution towards the downstream of the flame.

Second, as expected, the PDFs are wider in more intense turbulence, i.e. at higher Ka , cf. flames A, B, and C.

Third, while the probability of finding negative dilatation is low in flames IIS, A, and B, the PDF $P(\Theta^*)$ does not vanish at negative Θ^* in case C, thus indicating that the turbulence-controlled dilatation does play a role in flame C.

The role of turbulence-controlled dilatation at strong turbulence is further evidenced in Fig. 4, which reports various correlation coefficients $C_{a,b} = (\overline{ab} - \bar{a}\bar{b})/(\overline{a^2} \overline{b^2})^{1/2}$. In particular, Fig. 4a shows that, in flame H, L, IIS, A, or B, the correlation coefficient $C_{\Theta,c}$ between dilatation and combustion progress variable decreases monotonously with \bar{c} in the largest part of the mean flame brush with the exception of its trailing zones. This trend is associated with the fact that (i) appearance of the local flame in a point x close to the leading (trailing) edge of the mean flame brush causes a positive (negative) local fluctuation $c'(x,t)$ and (ii) combustion-induced dilatation is predominantly positive in these weakly and moderately turbulent flames. Accordingly, $C_{\Theta,c}$ is positive at $\bar{c} < c^*$ and negative at $\bar{c} > c^*$, with c^* being close to 0.5. However, such behaviour is not observed in the highly turbulent flame C, where $C_{\Theta,c}$ is close to zero at $\bar{c} < 0.3$, thus implying that other physical mechanisms (e.g. the influence of turbulence on molecular mixing) significantly affect dilatation in that zone. Moreover, in flame C, the coefficient $C_{\Theta,\dot{\omega}_T}$ decreases at $\bar{c} > 0.3$ eventually due to the rapid decay of turbulence, as seen in Fig. 1f. Due to this rapid decay, the turbulence-controlled dilatation effect pronounced in flame C becomes mitigated at $\bar{c} > 0.3$.

Figure 4b shows that the correlation coefficient C_{Θ,a_t} between dilatation and the local strain rate $a_t = -\mathbf{n} \cdot \nabla \mathbf{u}$ is about 0.4-0.5 in the largest parts of the IIS, A, and

B flame brushes, as well as in flame C provided that $\bar{c} > 0.3$. Here, $\mathbf{n} = -\nabla c/|\nabla c|$ designates the unit normal vector. This positive correlation is attributed to a decrease in the local flame thickness (and, hence, an increase in dilatation) in positively strained local flames. Such an effect is well known in the theory of strained laminar premixed flames⁸⁸ since the pioneering work by Klimov.⁸⁹ An increase in C_{Θ,a_t} with \bar{c} in the single-step-chemistry flames H and L is attributed to a more important role played by the local curvature (strain rate) at small (large, respectively) \bar{c} in these flames, as discussed elsewhere.⁴² However, in the leading zone ($\bar{c} < 0.3$) of flame C, the correlation coefficient is significantly lower than in other complex-chemistry flames, implying again that other physical mechanisms (e.g. the influence of turbulence on molecular mixing) significantly affect dilatation in that zone.

Figure 4c shows that the correlation coefficient C_{Θ,Ω_T} between dilatation and the local heat release rate $\Omega_T = \dot{\omega}_T/c_p$ is close to unity in the largest parts of the IIS, A, and B flame brushes with the exception of their trailing edges, as well as in flame C at $0.6 < \bar{c} < 0.85$. Such a strong correlation implies that the dilatation is mainly controlled by the combustion-induced thermal expansion in these complex-chemistry flames. In the leading zone of the C flame brush, however, the correlation coefficient is lower, again suggesting that other physical mechanisms (e.g. the influence of turbulence on molecular mixing) significantly affect dilatation in that zone. Note that, in the single-step-chemistry flames H and L, the coefficient C_{Θ,Ω_T} is lower, because dilatation and heat release rates peak at significantly different c (0.66 and 0.89, respectively) in the unperturbed laminar flames.

Figure 4d shows that the behaviour of the correlation coefficient $C_{\Theta,|\nabla c|}$ between dilatation and $|\nabla c|$ is similar to the behaviour of C_{Θ,Ω_T} , discussed above. The large value of $C_{\Theta,|\nabla c|}$ results directly from Eq. (9) that shows that $\Theta \propto |\nabla c|$. Lower values of $C_{\Theta,|\nabla c|}$ obtained in the leading zone of flame C indicate that the influence of turbulence on S_d (or, more specifically, on the molecular mixing term in the definition of S_d) plays an important role in that zone, in line with the above discussion of other results reported in Fig. 4. Moreover, these results reveal a way that flame propagation resists to turbulent perturbations, an effect that, to our knowledge, has not yet been discussed in the literature. In other words, if turbulence strongly perturbs a flame locally and makes S_d negative in the flame preheat zone, the turbulence-controlled dilatation increases the local dissipation rate, thus mitigating the local turbulence.

Overall, the present DNS data (in particular, data obtained from flame C) indicate that the turbulence-controlled dilatation may play a role even in highly turbulent flames and, therefore, may notably contribute to the total dissipation rate. This issue definitely requires further DNS research into premixed turbulent flames characterized by Karlovitz numbers higher than the value of $Ka = 126$, which was reached in case C.

Note that if Ka is increased by decreasing the integral length scale L , the mean flame brush thickness δ_f may be decreased. Such an effect is evident in flame C when compared to flames A and B, as discussed elsewhere.⁶³ In particular, in case C, the time-averaged $\delta_f = 1/\max\{|\nabla c|\}$ (i) is smaller by

FIG. 5. Mean dilatation $\nabla \cdot \bar{\mathbf{u}}$ normalized using $(\sigma - 1)S_L/\delta_L$ vs. Reynolds-averaged combustion progress variable.

FIG. 6. Magnitude $(\nabla \cdot \mathbf{u}')^2$ of dilatation fluctuations, normalized using $(\sigma - 1)^2 S_L^2/\delta_L^2$, vs. Reynolds-averaged combustion progress variable.

a factor of about 3.5 than in case A or B and (ii) is approximately equal to $3\delta_L$. The decrease in δ_L results in increasing the mean dilatation $\nabla \cdot \bar{\mathbf{u}}$. Indeed, Fig. 5 shows that $\nabla \cdot \bar{\mathbf{u}}$ is significantly larger in case C when compared to other five cases.

Figure 6 shows that the magnitude $(\nabla \cdot \mathbf{u}')^2$ of dilatation fluctuations is significantly larger in flame C when compared to other five cases. However, this difference is related more to the turbulence-controlled dilatation rather than to the small thickness δ_L of flame C.

D. Influence of diffusive-thermal effects on dilatation

When analyzing results plotted in Fig. 1f, one might attribute substantial values of dilatational dissipation observed at the leading edge of the mean C flame brush to diffusive-thermal effects, which are discussed in detail elsewhere.^{69–71} Such effects are well known to cause significant changes in the local equivalence ratio and enthalpy (when compared to the reference unperturbed laminar flame) due to imbalance of local heat and species fluxes from/to reaction zones wrinkled and strained by turbulent eddies. As a result, in lean hydrogen-air turbulent flames, local reaction rates, $|\nabla c|$, and combustion temperature can be increased if the local flame curvature or strain rate is positive.⁸⁸ Consequently, the local dilatation can also be increased.

Such effects are revealed in Fig. 7, which reports PDFs $P(\Theta^*)$ of the normalized dilatation conditioned to various ratios of $\Omega_T(x, t)/\max\{\Omega_T(x, t)\}$, with the maximum (over the entire computational domain and various instants) heat release rates $\max\{\Omega_T(x, t)\}$ being different due to different magnitudes of the diffusive-thermal effects. More specifically, $\max\{\Omega_T(x, t)\}$ is significantly increased by Ka , i.e. $\max\{\Omega_T(x, t)\} = 8600, 13\,500$ and $30\,000$ ($\text{g} \cdot \text{K}/(\text{cm}^3 \cdot \text{s})$) in flames A, B, and C, respectively. Figure 7 shows that a higher rate $\Omega_T(x, t)$ is statistically linked with a higher normalized dilatation Θ^* , with the highest local values of $\Omega_T(x, t)$ being accompanied by the highest local values of Θ^* , as for $c = 0.75$ and 0.90 . The effect is strongly pronounced in case C, where Θ^* can be as large as 12. Note that an increase in Θ^* from

FIG. 7. Probability density functions $P(\Theta^*)$ of the normalized dilatation conditioned to various ratios of $\Omega_T(x, t)/\max\{\Omega_T(x, t)\}$, specified in legends. The PDFs have been sampled from the entire computational domains. (a) Bangalore flame IIS, (b) KAUST flame A, (c) KAUST flame B, (d) KAUST flame C.

FIG. 8. (a) Probability density functions $P(\delta_L^{-1} \nabla \cdot \mathbf{n})$ of the normalized curvature extracted from different zones of the C flame brush, characterized by the mean values of the combustion progress variable specified in legends. (b) Variations in the probabilities of $\delta_L^{-1} \nabla \cdot \mathbf{n} > 1$ and $\delta_L^{-1} \nabla \cdot \mathbf{n} < -1$ in the flame brush.

FIG. 9. Extreme (over transverse plane and time) values of (a) local heat release rate normalized using the peak heat release rate in the unperturbed laminar flame and (b) normalized dilatation Θ^* vs. mean combustion progress variable. In the right panel, both positive and negative extreme values are plotted using the same line style for each flame, but different colors (red and black, respectively).

unity to 12 (Fig. 7d) yields an increase in the local dilatational dissipation rate by two orders of magnitude.

Such local perturbations are expected at low values of \bar{c} , because positively curved reaction zones are localized at the leading edge of the mean flame brush. Indeed, Fig. 8a shows that the PDF of local curvature $\nabla \cdot \mathbf{n}$ normalized using the laminar flame thickness δ_L is shifted to positive values at the leading edge ($\bar{c} = 0.05$) when compared to the middle of the flame brush ($\bar{c} = 0.5$) or its trailing edge ($\bar{c} = 0.95$). As a result, the probability of $\delta_L^{-1} \nabla \cdot \mathbf{n}$ being larger than unity is the highest at low \bar{c} and decreases with increasing \bar{c} (Fig. 8b). On the contrary, the probability of $\delta_L^{-1} \nabla \cdot \mathbf{n} < -1$ is increased by \bar{c} .

While results reported in Figs. 7 and 8 appear to be consistent with the assumption that the diffusive-thermal effects contribute substantially to significant values of dilatational dissipation rate observed in Fig. 1f at small \bar{c} , inspection of other DNS data does not support this hypothesis. For instance, Fig. 9 shows that the maximum (over transverse plane and time) values of heat release rate and dilatation (i) depend weakly on the mean combustion progress variable in flames A and B and (ii) peak at values of \bar{c} that are larger than values of \bar{c} associated with the highest dilatational dissipation rate in flame C. The decrease in the extreme values of the normalized Ω_T and Θ^* with the mean combustion progress variable is attributed to the rapid turbulence decay in case C, as seen in Fig. 1f.

Moreover, Fig. 10 indicates that the probability of finding a local heat release rate larger than its maximum value in the unperturbed laminar flame peaks in the middle of the flame brush, rather than at low \bar{c} . Furthermore, Fig. 11 shows that a ratio of dilatational and solenoidal dissipation rates (the same rates are plotted in Fig. 1f in another format) does not exhibit a peak at the leading edge of the flame brush in case C, but is increased with \bar{c} up to $\bar{c} \approx 0.8$. This increase can be attributed to the turbulence decay, because the dilatational dissipation rate plays a more important role at lower Ka , as shown in Fig. 1f.

Thus, results reported in Figs. 10 and 11 imply that the sig-

FIG. 10. Probability of finding a local heat release rate larger than its maximum value in the unperturbed laminar flame vs. mean combustion progress variable.

FIG. 11. Ratio of dilatational and solenoidal dissipation rates vs. mean combustion progress variable in flame C.

nificant dilatational dissipation rates encountered at low \bar{c} in case C are unlikely to be caused by the diffusive-thermal effects. Indeed, since the mean thickness of flame C is comparable with the laminar flame thickness ($\delta_f \approx 3\delta_L$), the probability that reaction zones perturbed by turbulent eddies appear at a low \bar{c} is very low. On the contrary, turbulence-controlled dilatation can be observed in preheat zones at a low \bar{c} and a curve plotted in black dotted lines in Fig. 9b does show that the magnitude of negative (turbulence-controlled) dilatation is highest at low \bar{c} in case C. Accordingly, the significant dilatational dissipation rates found at low \bar{c} in case C are associated with the influence of turbulence on molecular mixing in the preheat zones, rather than with the diffusive-thermal effects. Nevertheless, such effects could play a role in the middle of the flame brush, where (i) the maximum values of the local heat release rate and dilatation are still high (Fig. 9) and (ii) the probability of finding Ω_T larger than its maximum value in the unperturbed laminar flame peaks (Fig. 10). This issue requires further study and will be a subject for future research.

IV. CONCLUSIONS

DNS data obtained by three independent research groups using different numerical codes and methods (e.g., single-step chemistry and complex chemistry flames) from six different premixed turbulent flames associated with flamelet, thin reaction zone, and broken reaction zone regimes of turbulent burning were analyzed to evaluate total, solenoidal, and dilatational dissipations. Results show that dilatational dissipation can be larger than solenoidal dissipation in the flamelet regime and is also significant even in the thin reaction zone regime.

Moreover, certain physical arguments and numerical results imply that dilatational dissipation could play a role even in highly turbulent flames due to the influence of turbulence on molecular mixing in the local flame zones characterized by negligible heat release rate. In particular, due to this physical mechanism, local dilation can be negative and have large magnitude in the leading zone of the highly turbulent flame C ($Ka > 100$). As a result, a ratio of dilatational and solenoidal dissipations does not vanish in that zone, but stays close to 0.15. Moreover, while local dilatation and heat release rate correlate very well in the complex-chemistry flames IIS, A, and B associated with the flamelet and thin reaction zone regimes of premixed turbulent burning, such a correlation is substantially less pronounced at low \bar{c} in the complex-chemistry flame C characterized by the highest Karlovitz number, thus, indicating again importance of the turbulence-controlled dilatation in that highly turbulent flame.

DNS data obtained from four lean hydrogen-air flames also show that local heat release rate and dilatation can reach values that are significantly (by an order of magnitude in case C)

larger than the peak values of these quantities in the unperturbed laminar flames, with the effect magnitudes being increased by Karlovitz number. These findings are attributed to local heating and enrichment of reacting mixture due to imbalance of molecular fluxes of reactants and heat to and from, respectively, reaction zones wrinkled and strained by turbulent eddies. Such effects can also contribute to a substantial role played by dilatational dissipation in premixed turbulent flames.

To our knowledge, the present study provides the first evidence of the importance of dilatational dissipation in premixed turbulent flames characterized by low Mach numbers. In addition, the study shows that the influence of combustion-induced thermal expansion on dissipation rate is not limited to an increase in the mixture viscosity by the temperature.

A substantial role played by dilatational dissipation in premixed turbulent flames casts doubts on the direct application of conventional constant-density turbulence models for simulations of premixed burning. To further investigate dilatation and dilatational dissipation in premixed turbulent flames, a parametric DNS study aimed at exploring the function f on the right hand side of Eq. (5) appears to be of interest. To extend the range of considered parameters, such a study could be performed in the case of a single-step chemistry. Moreover, term-by-term analysis of the exact equation for dilatation appears to be of interest also and will be the subject of future work.

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Data availability statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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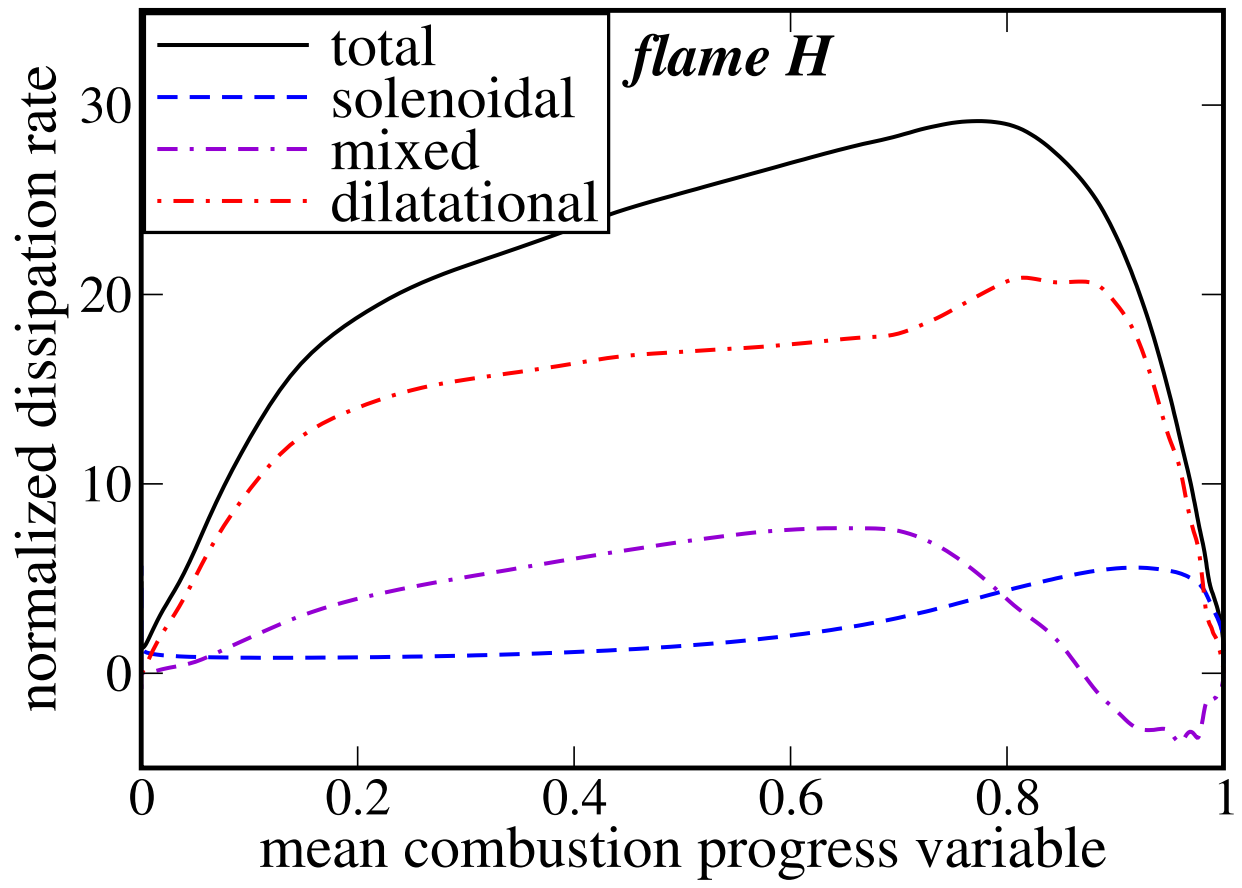
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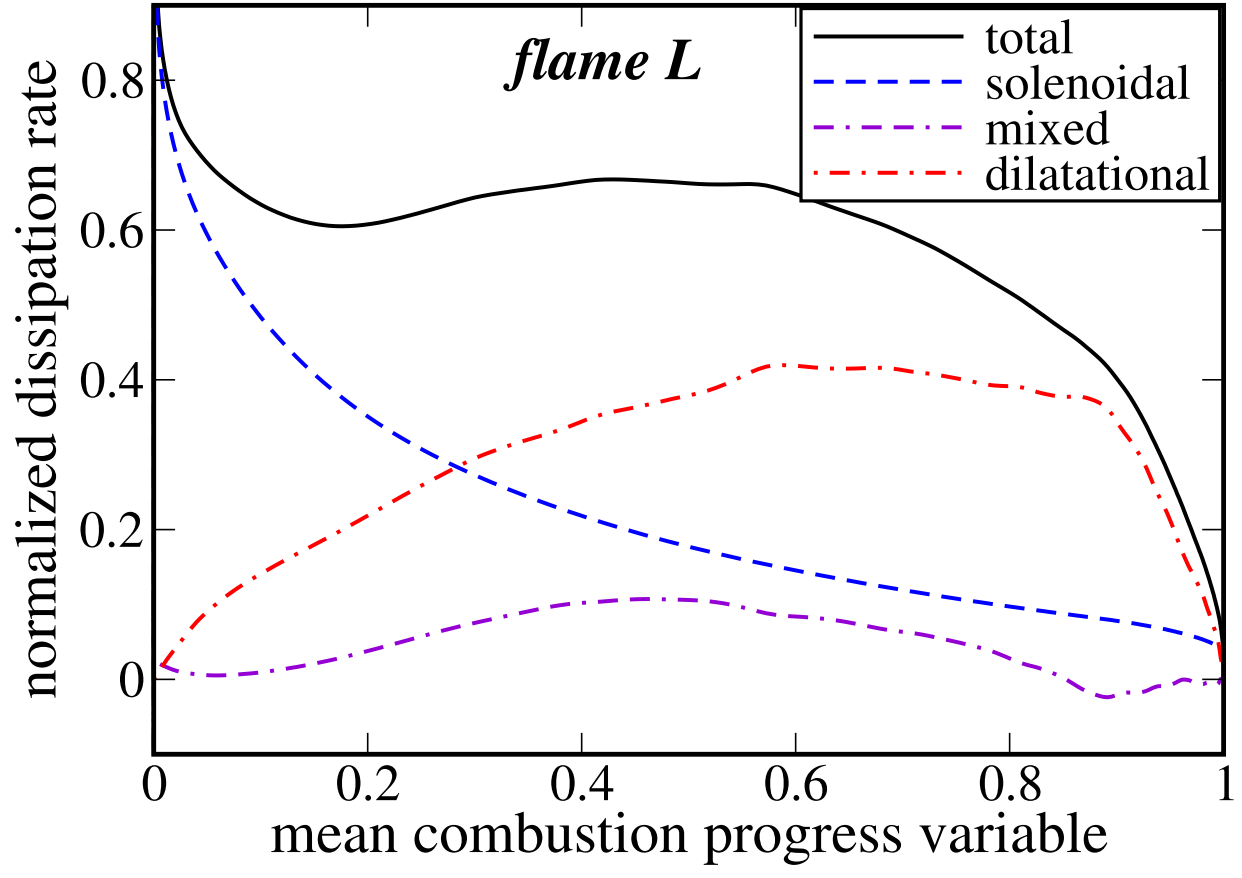
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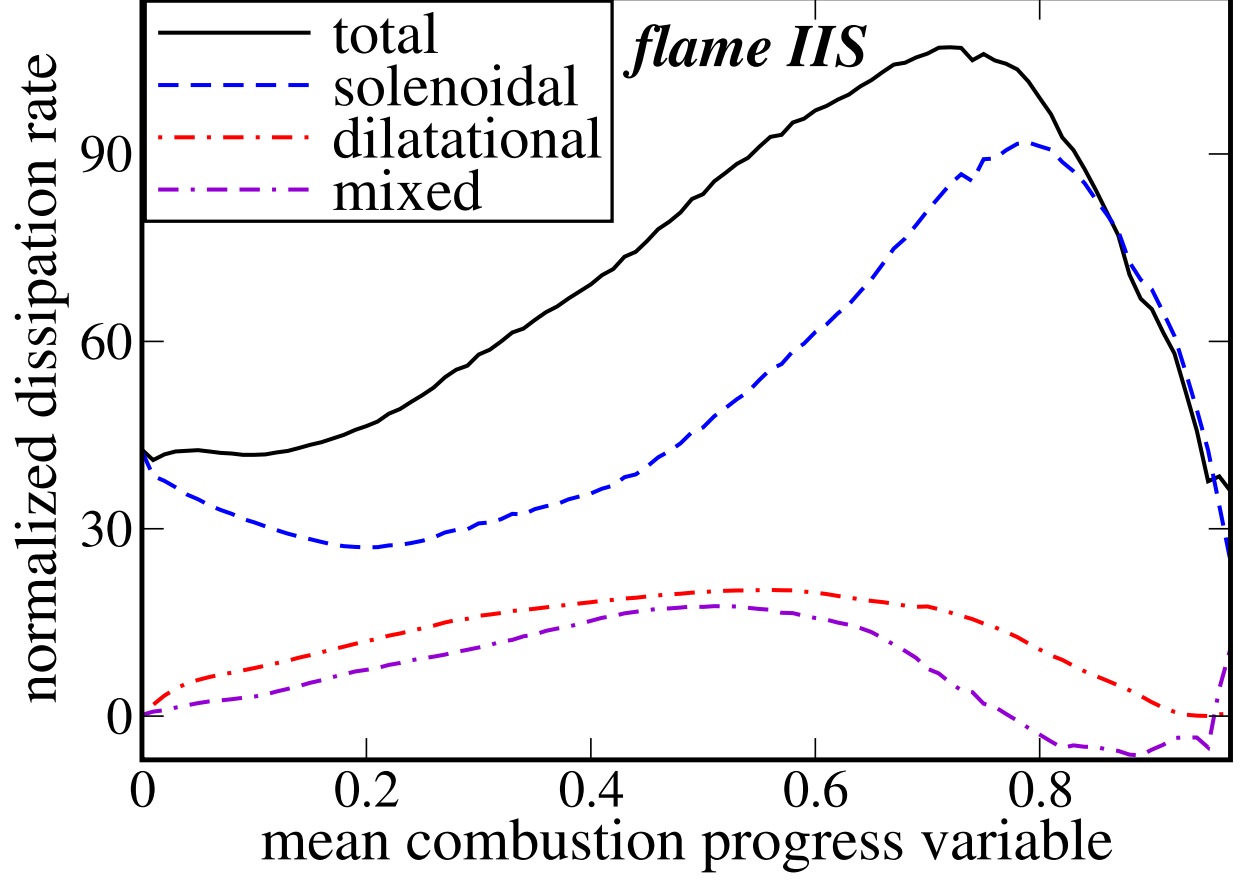
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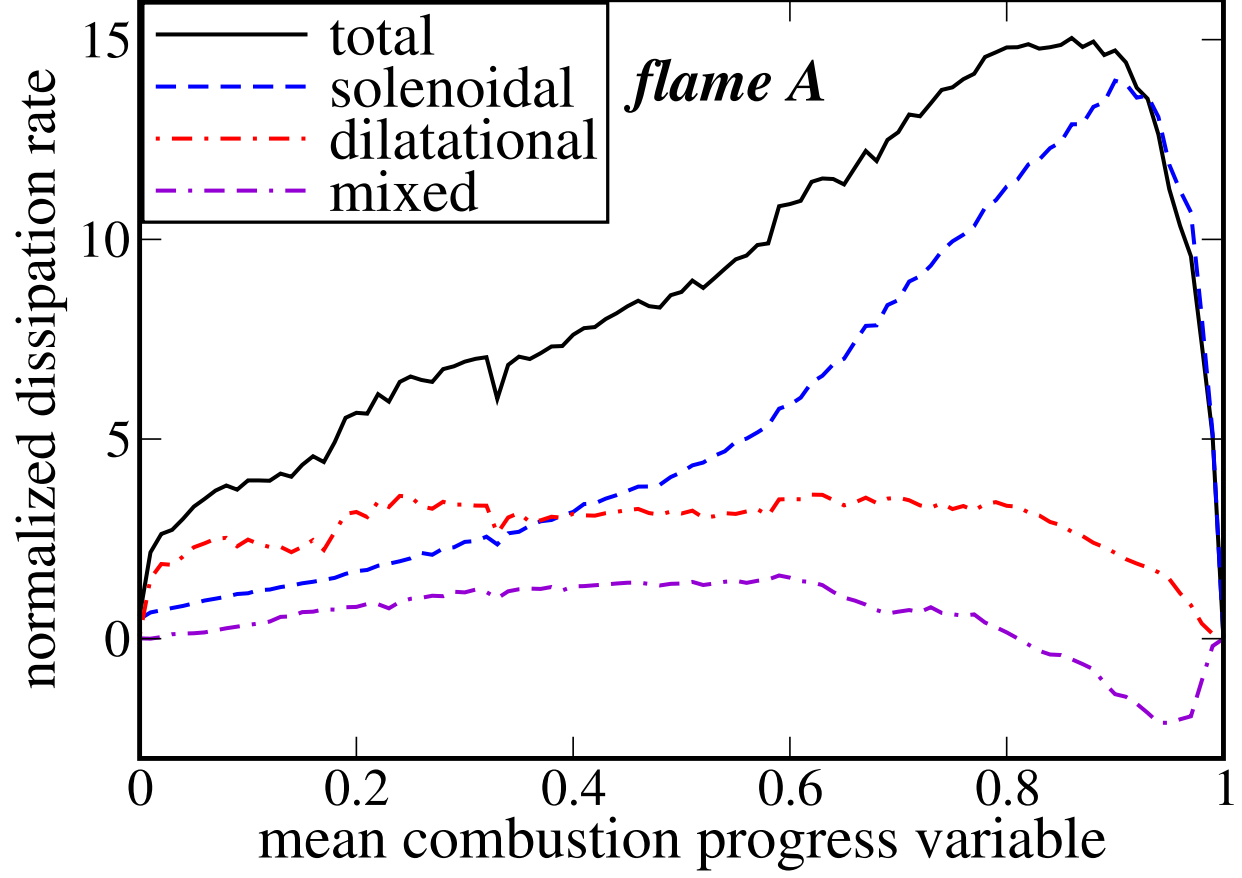
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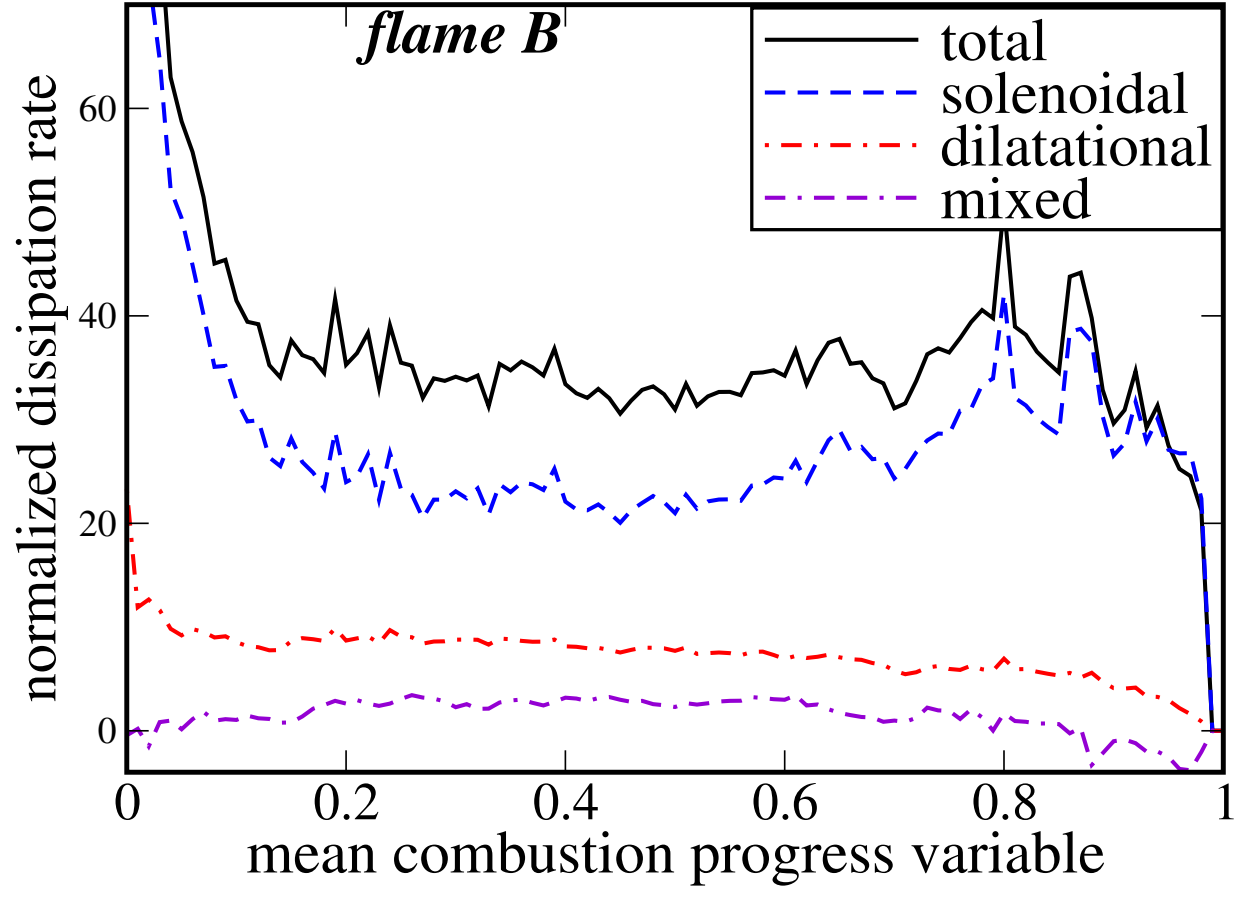


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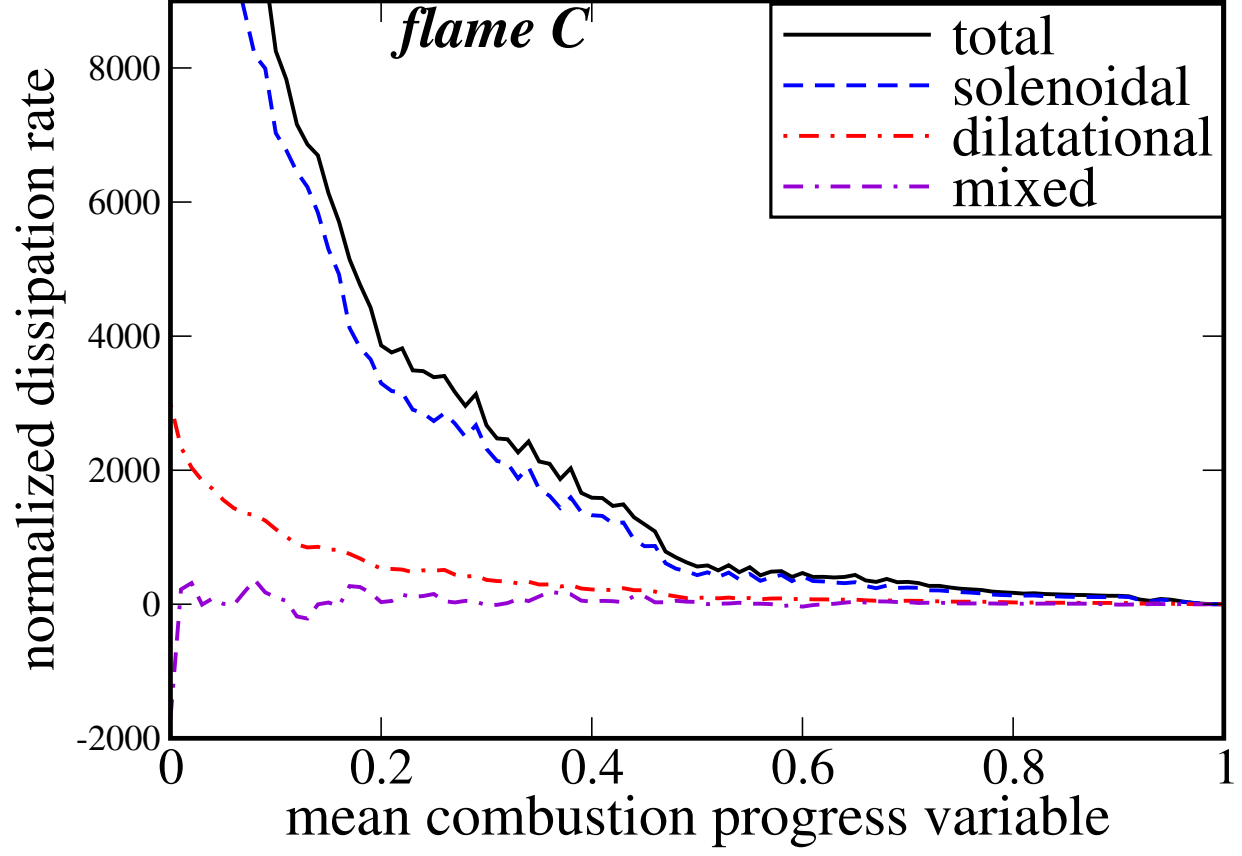


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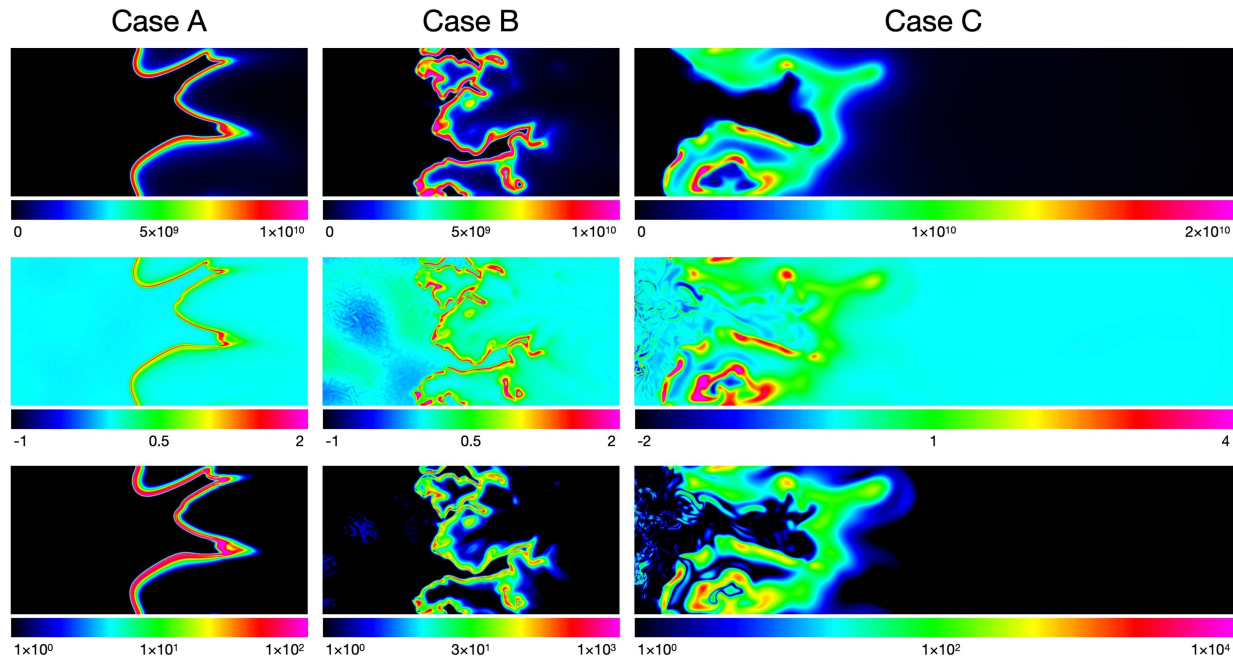
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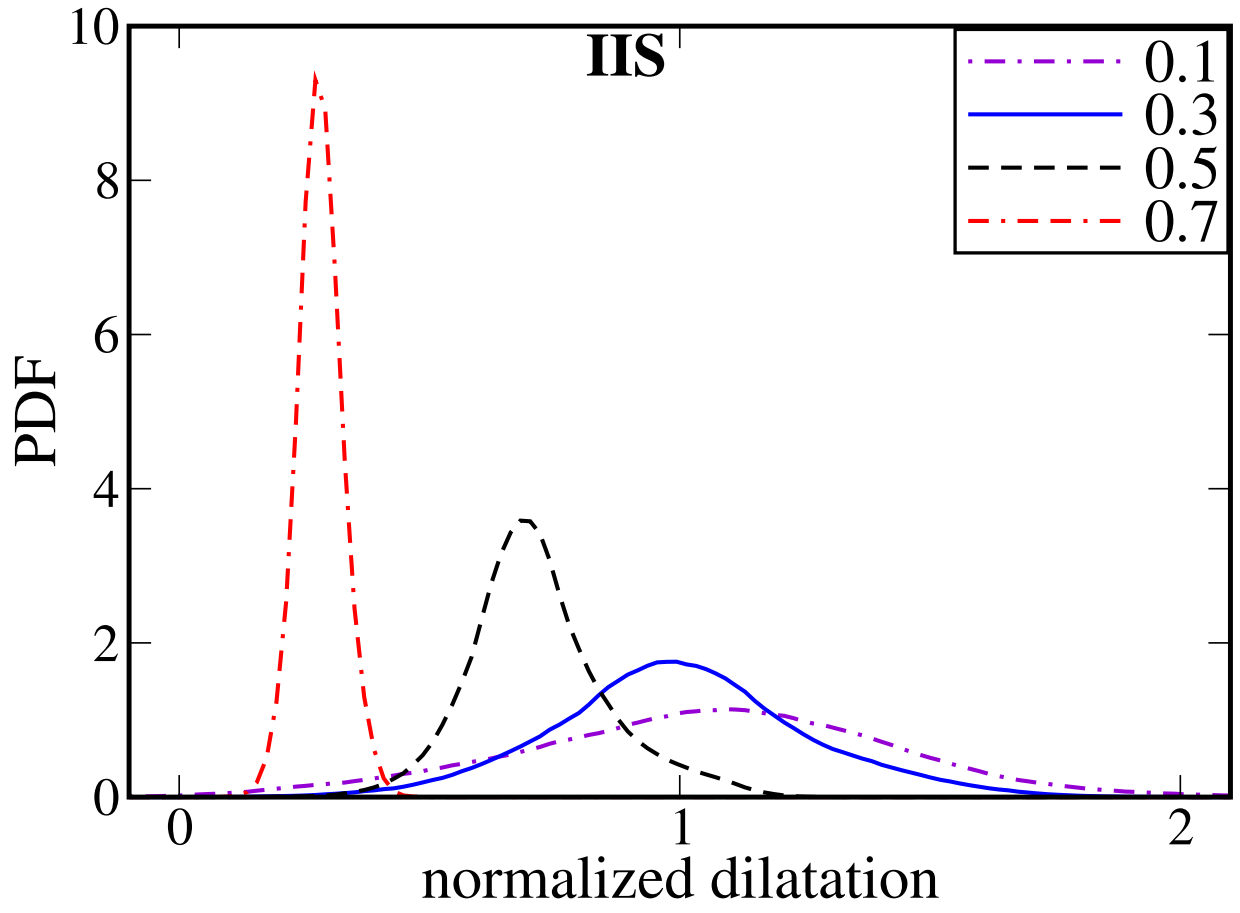
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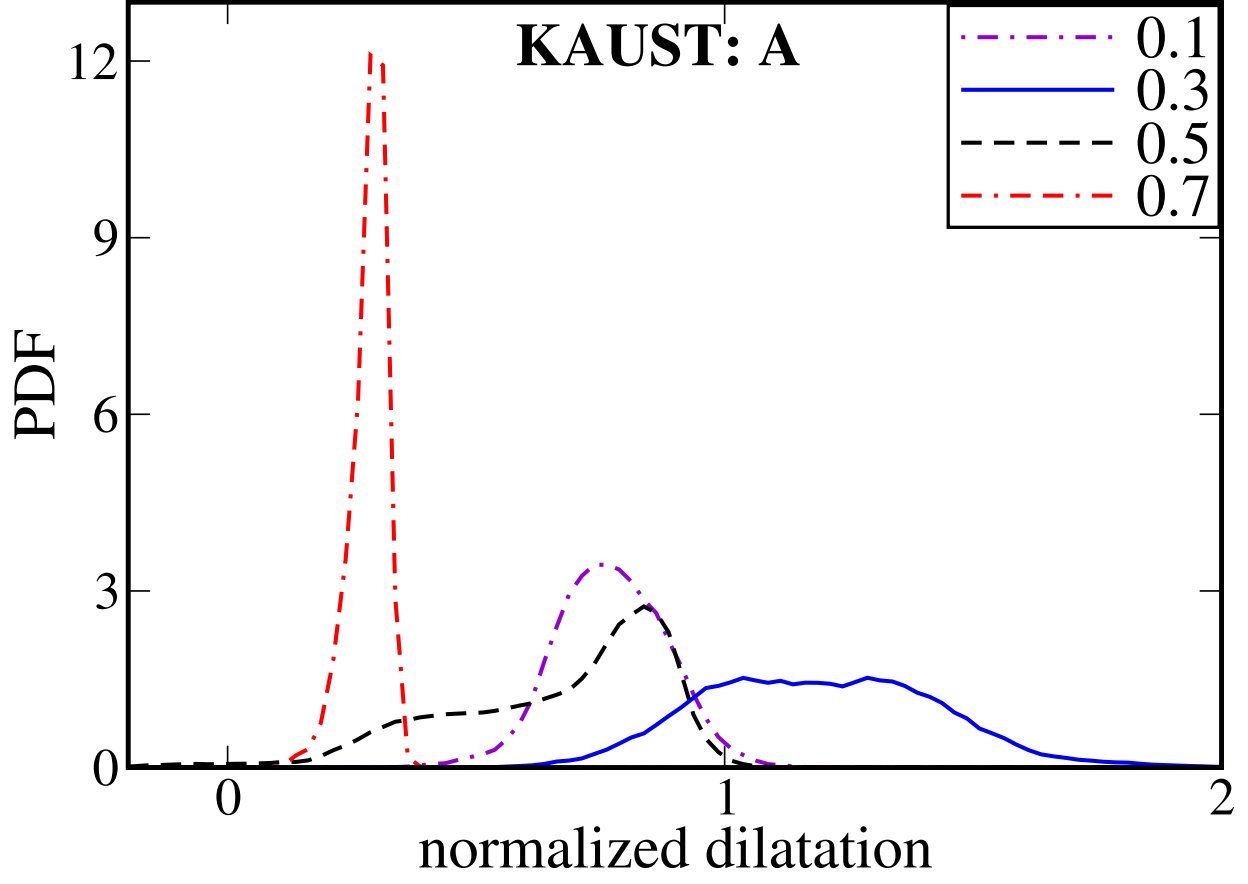
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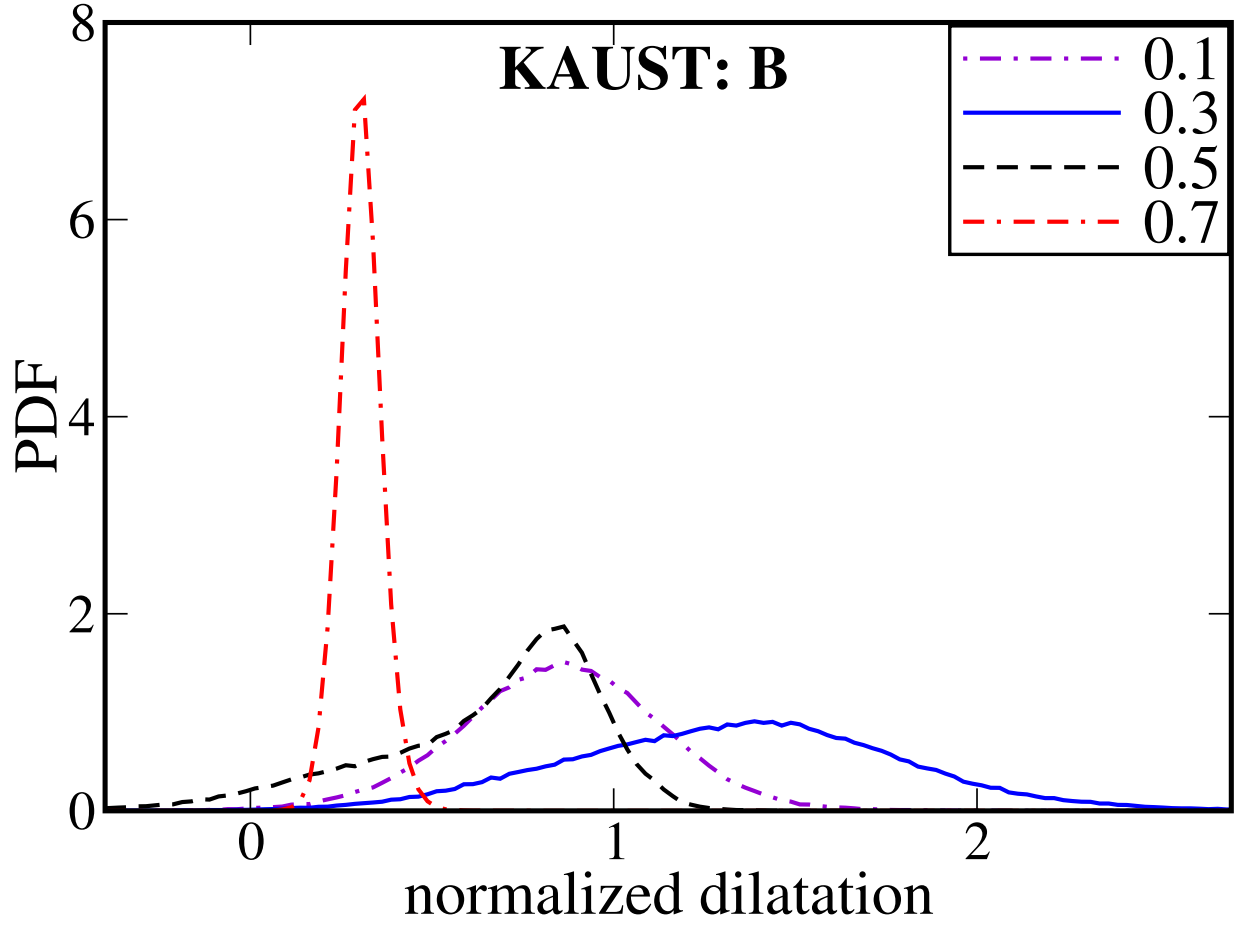
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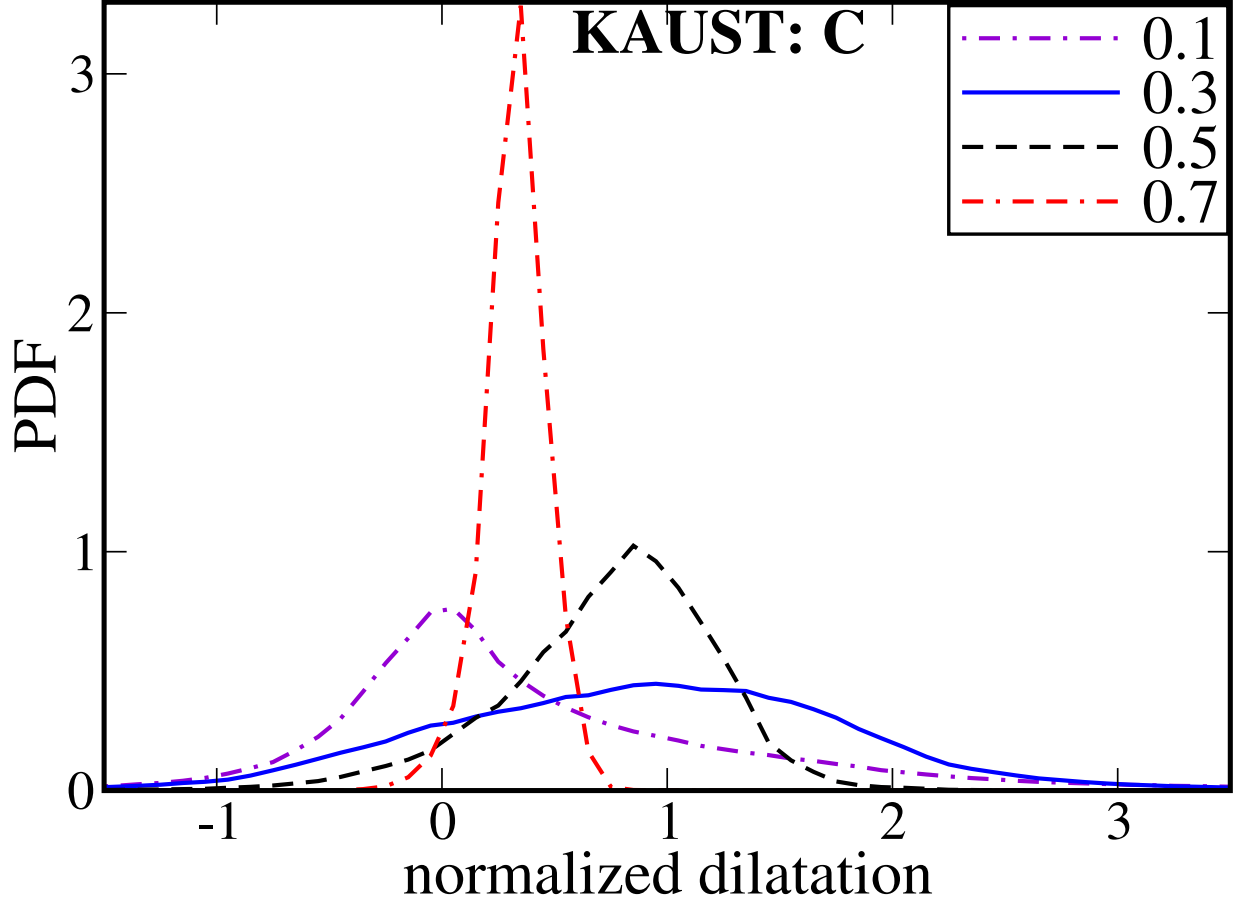
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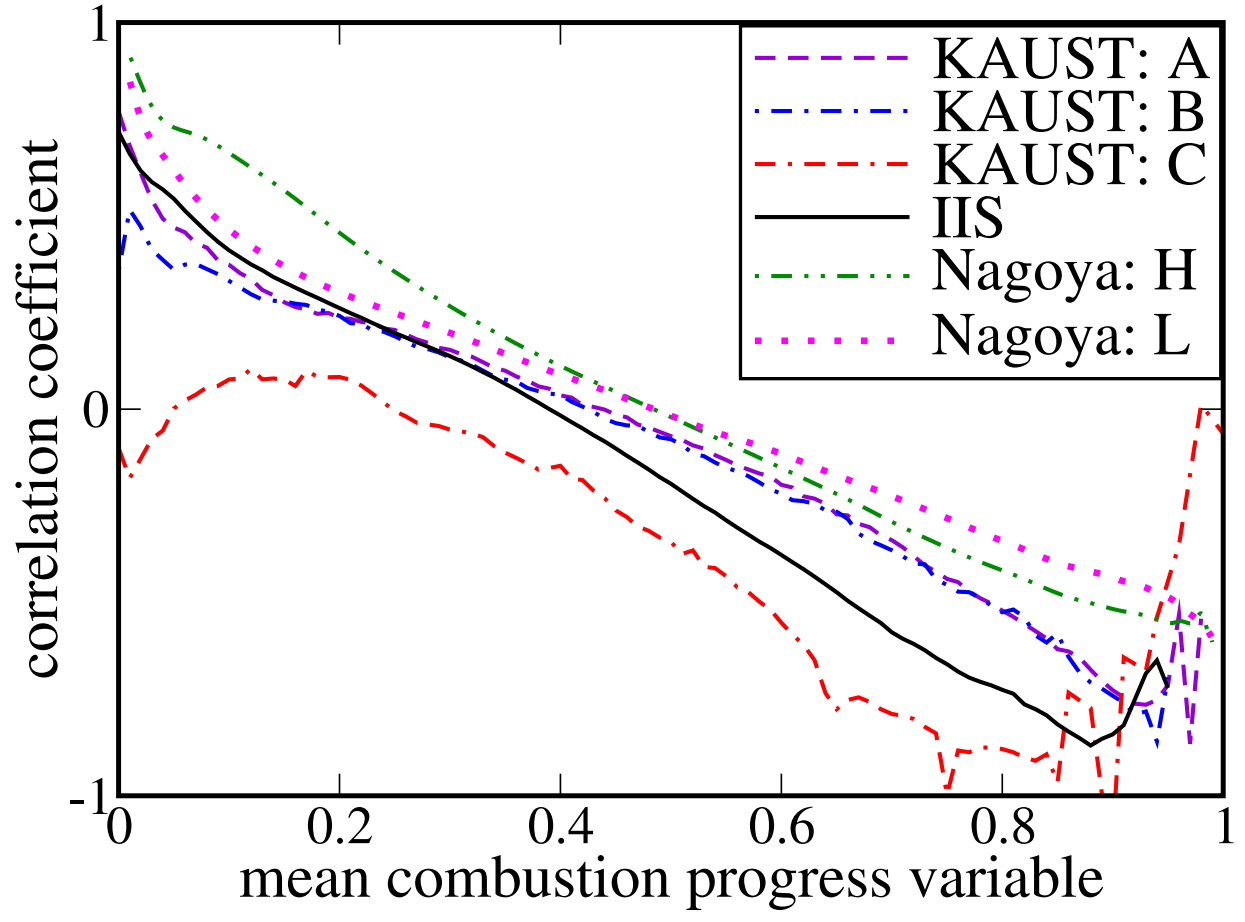
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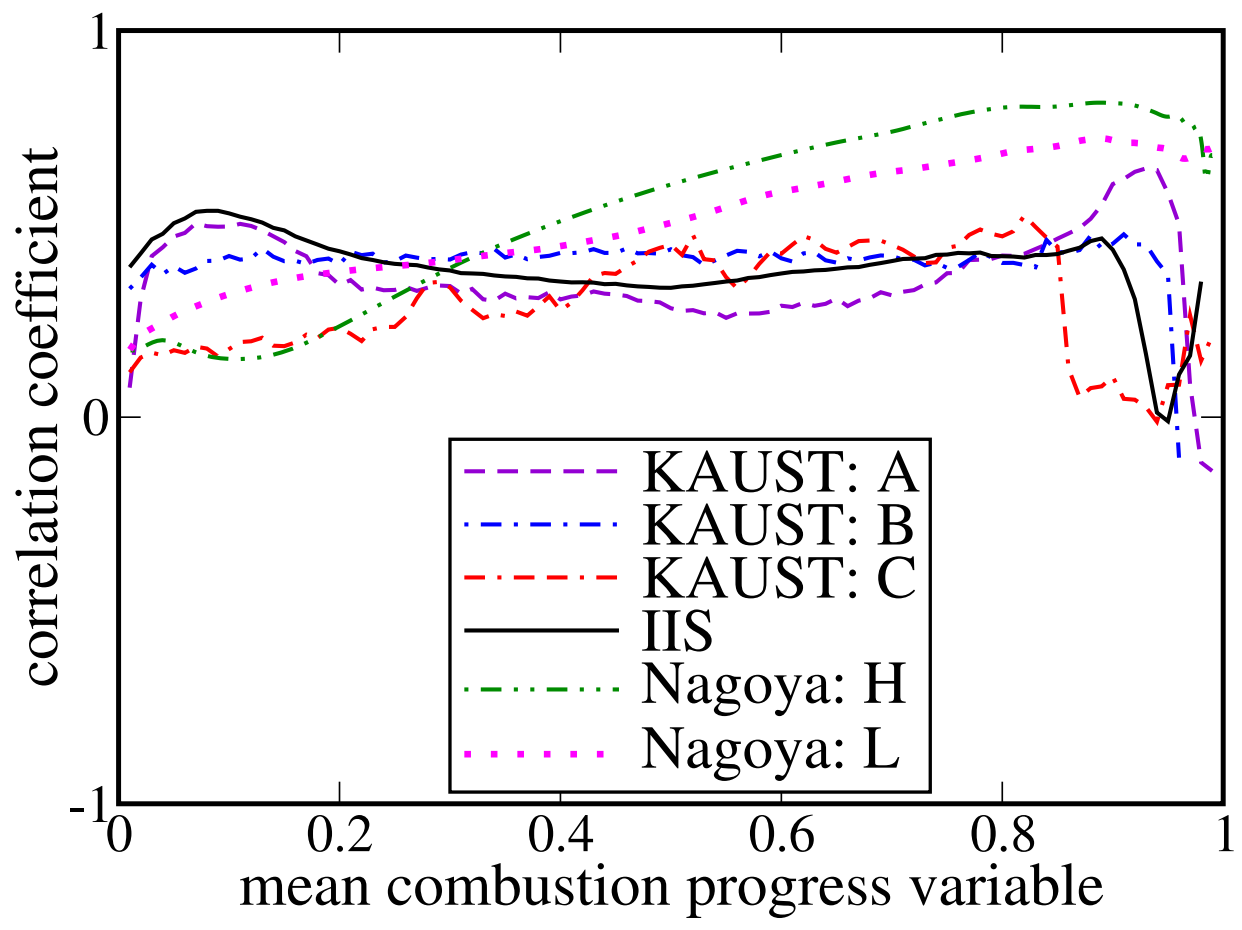


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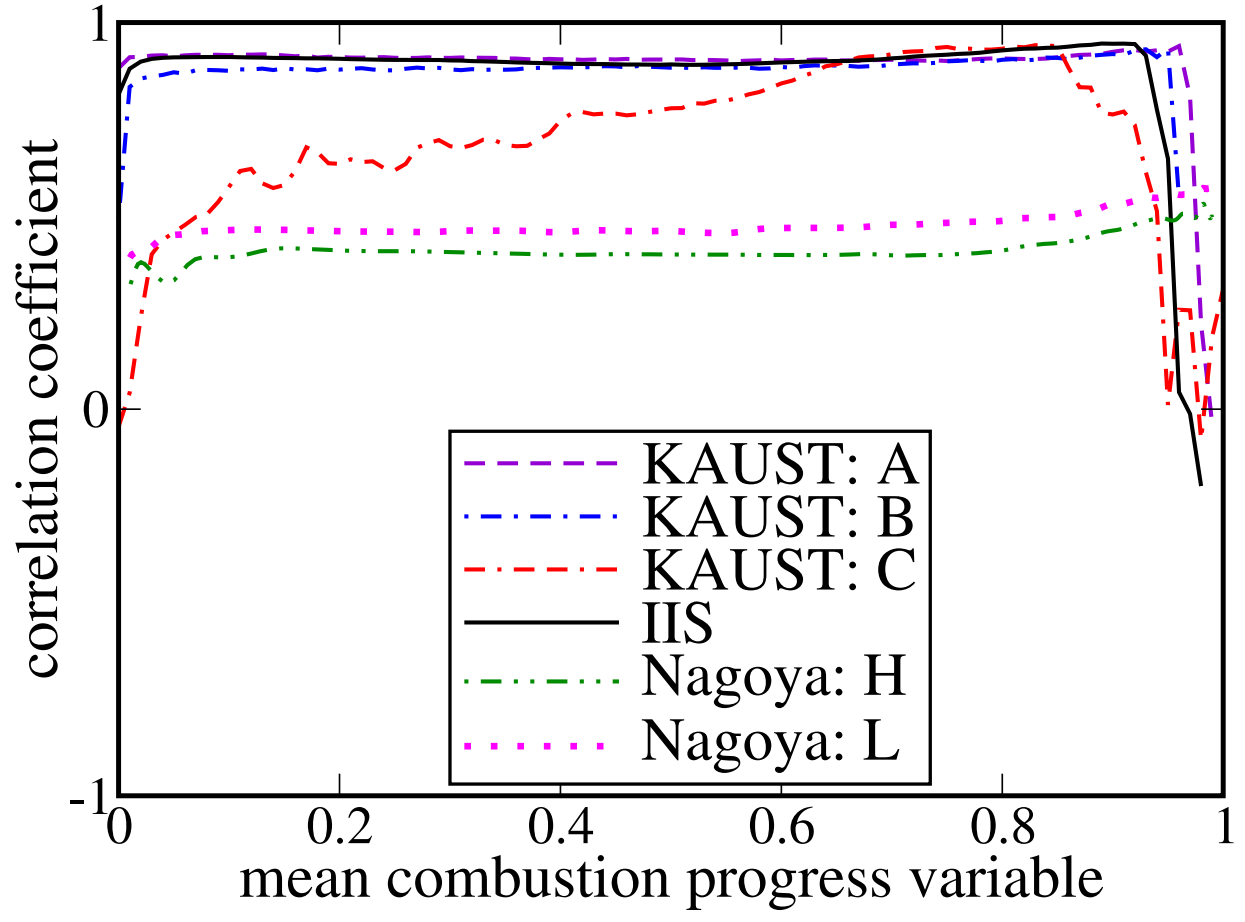


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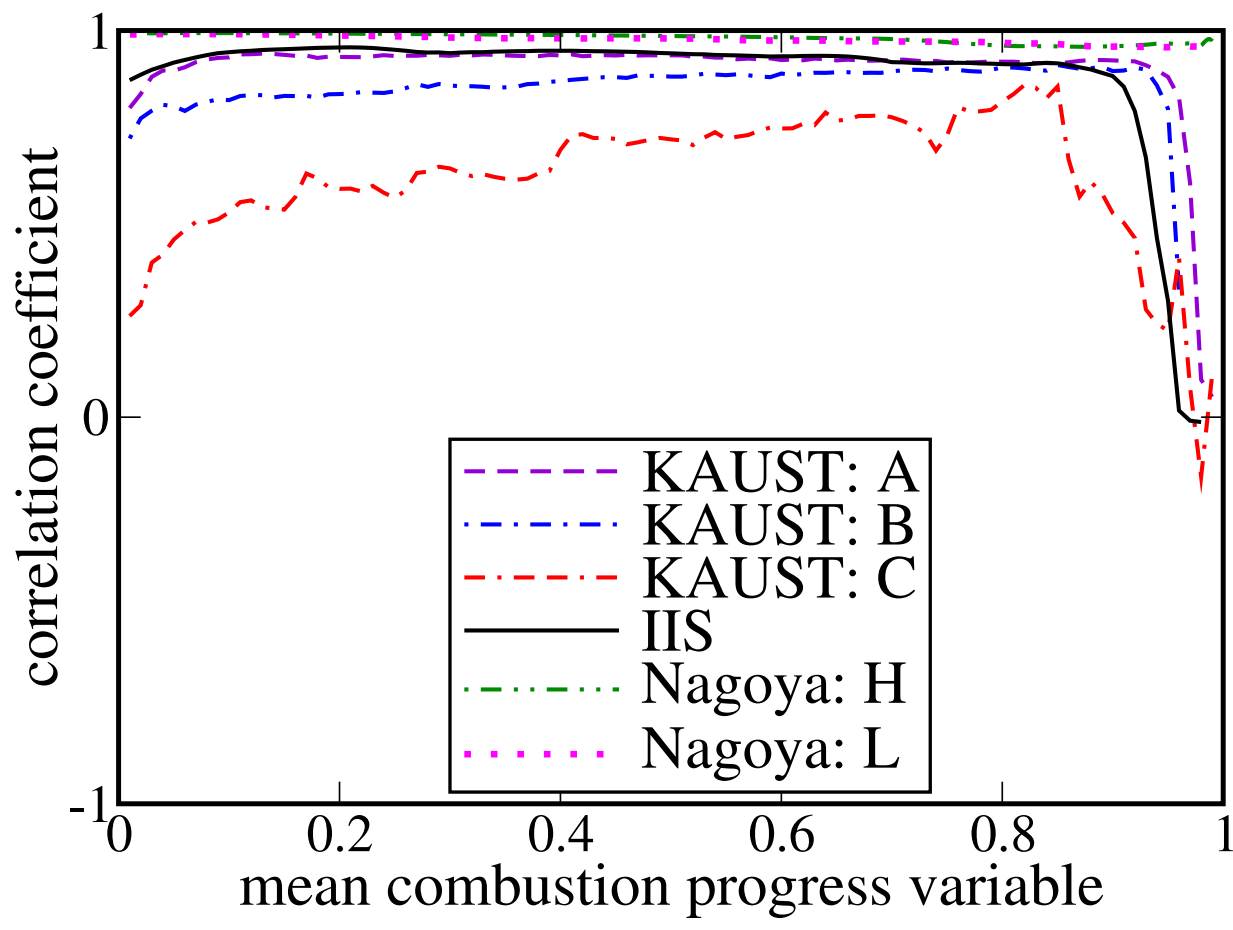
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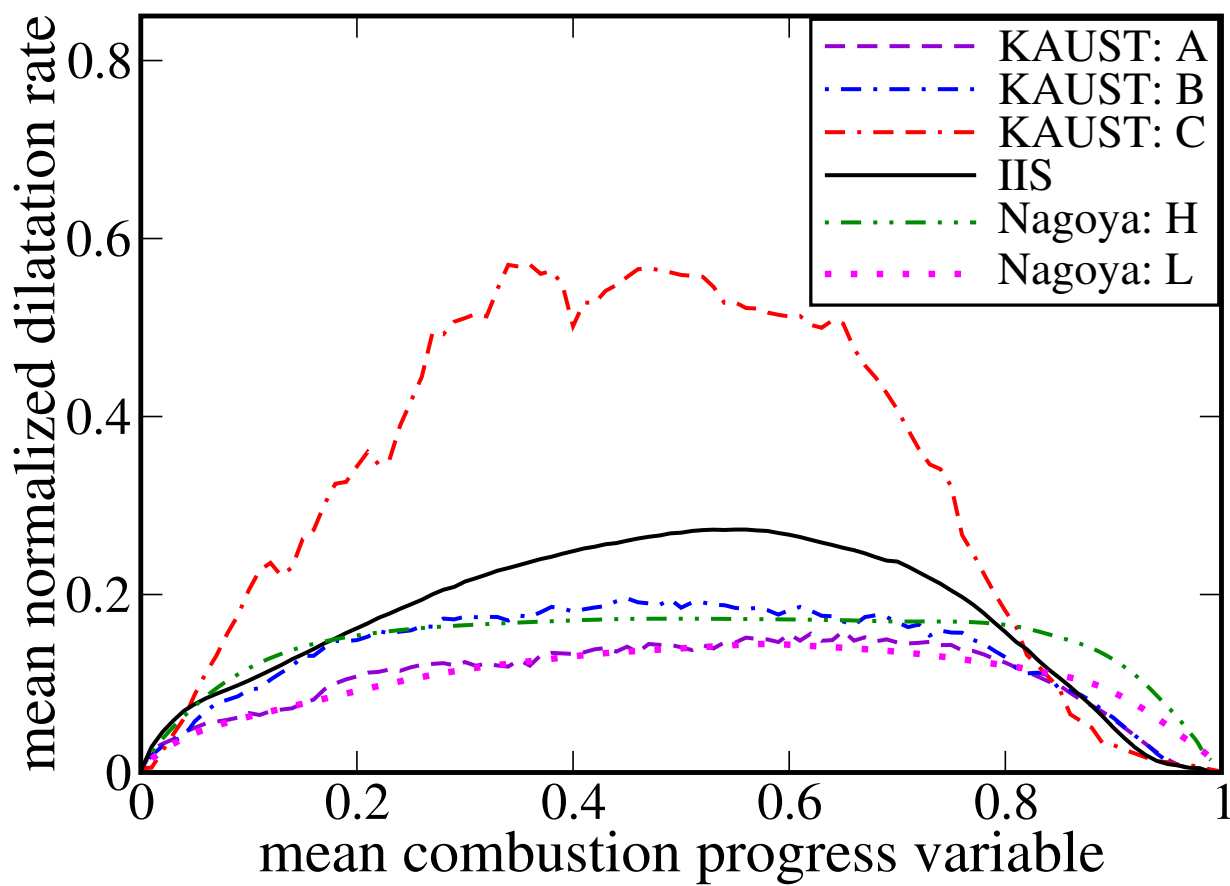


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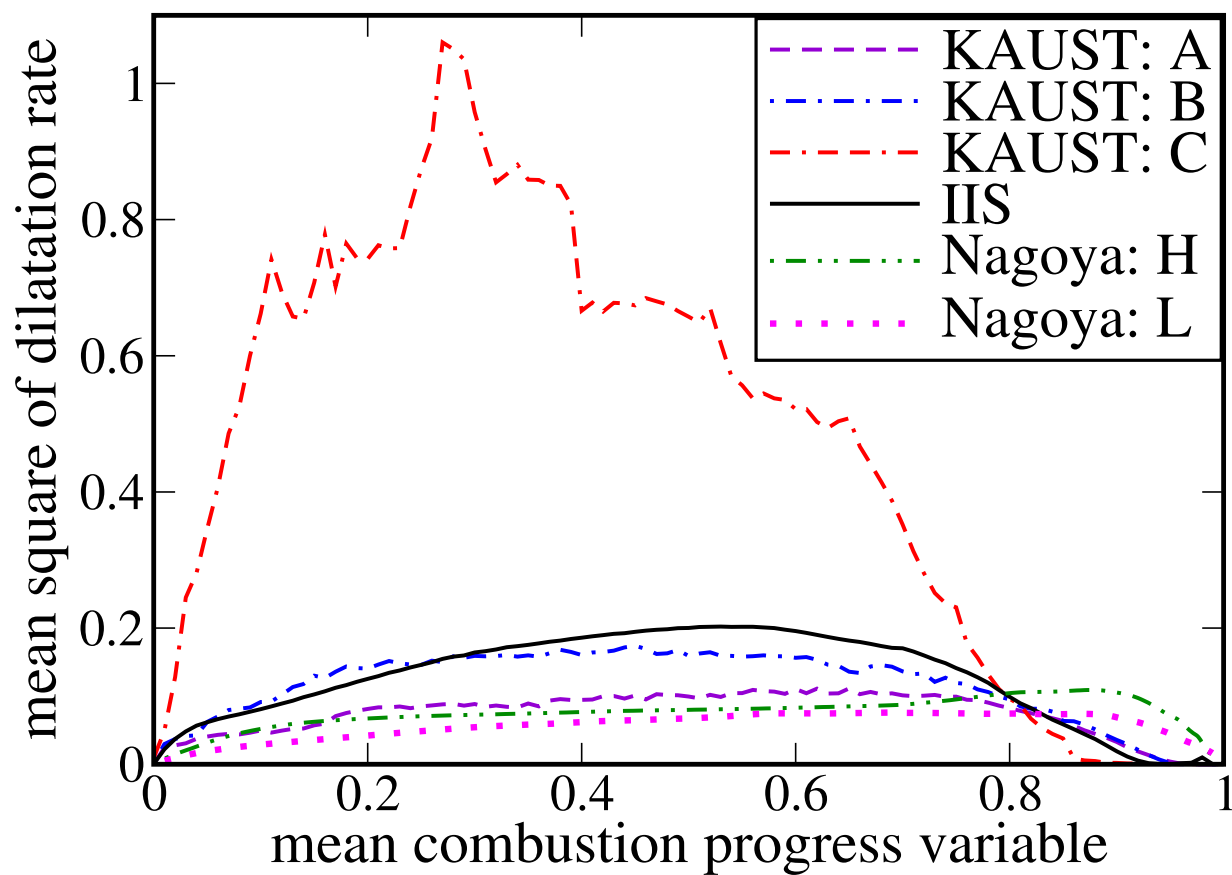


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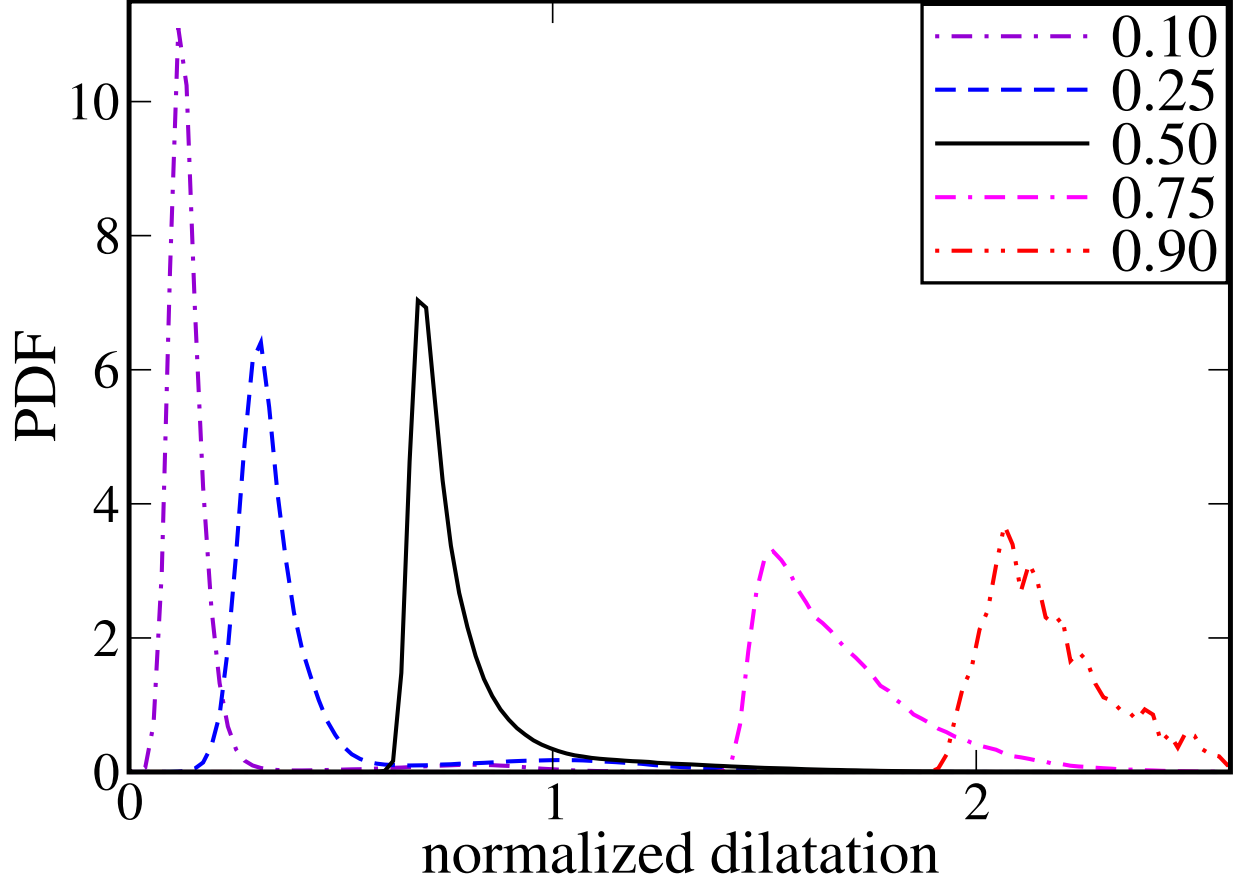
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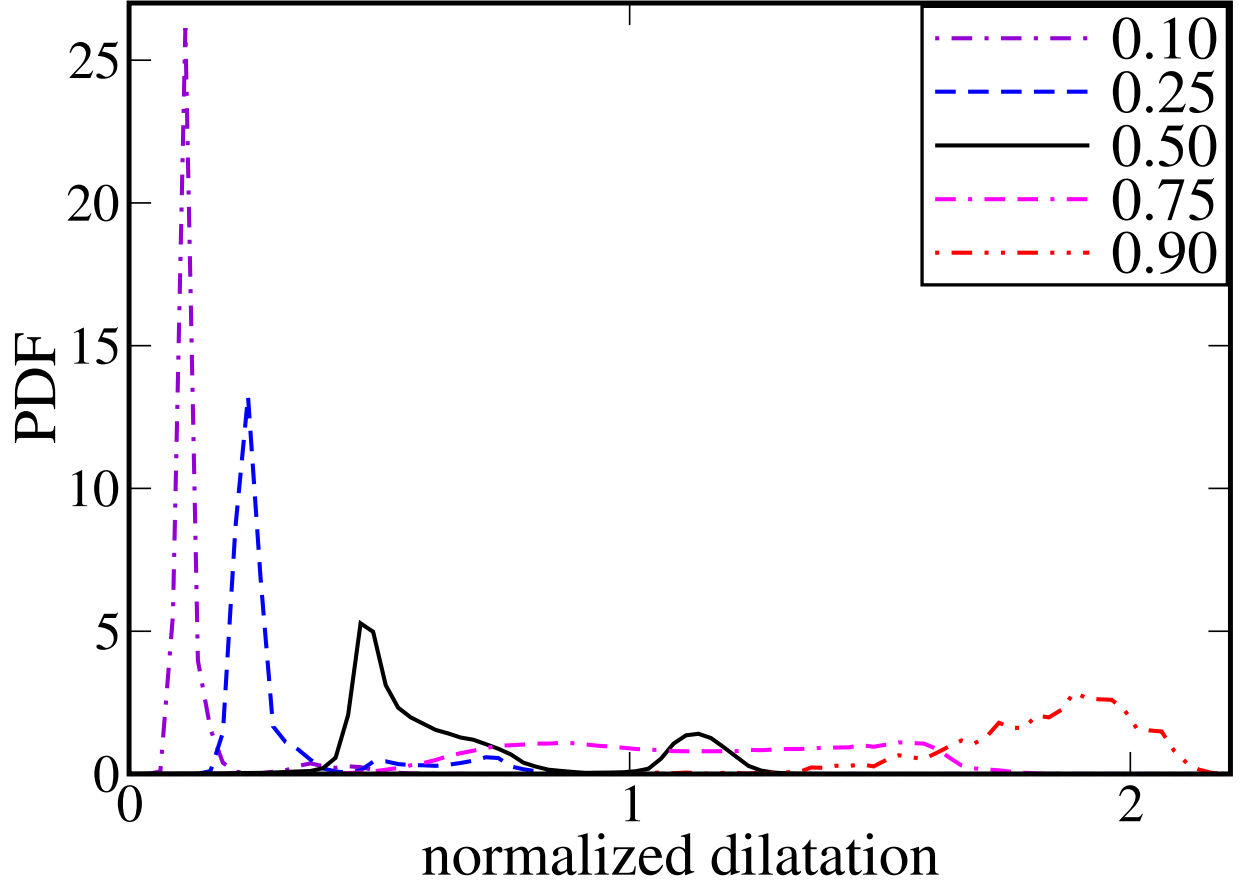
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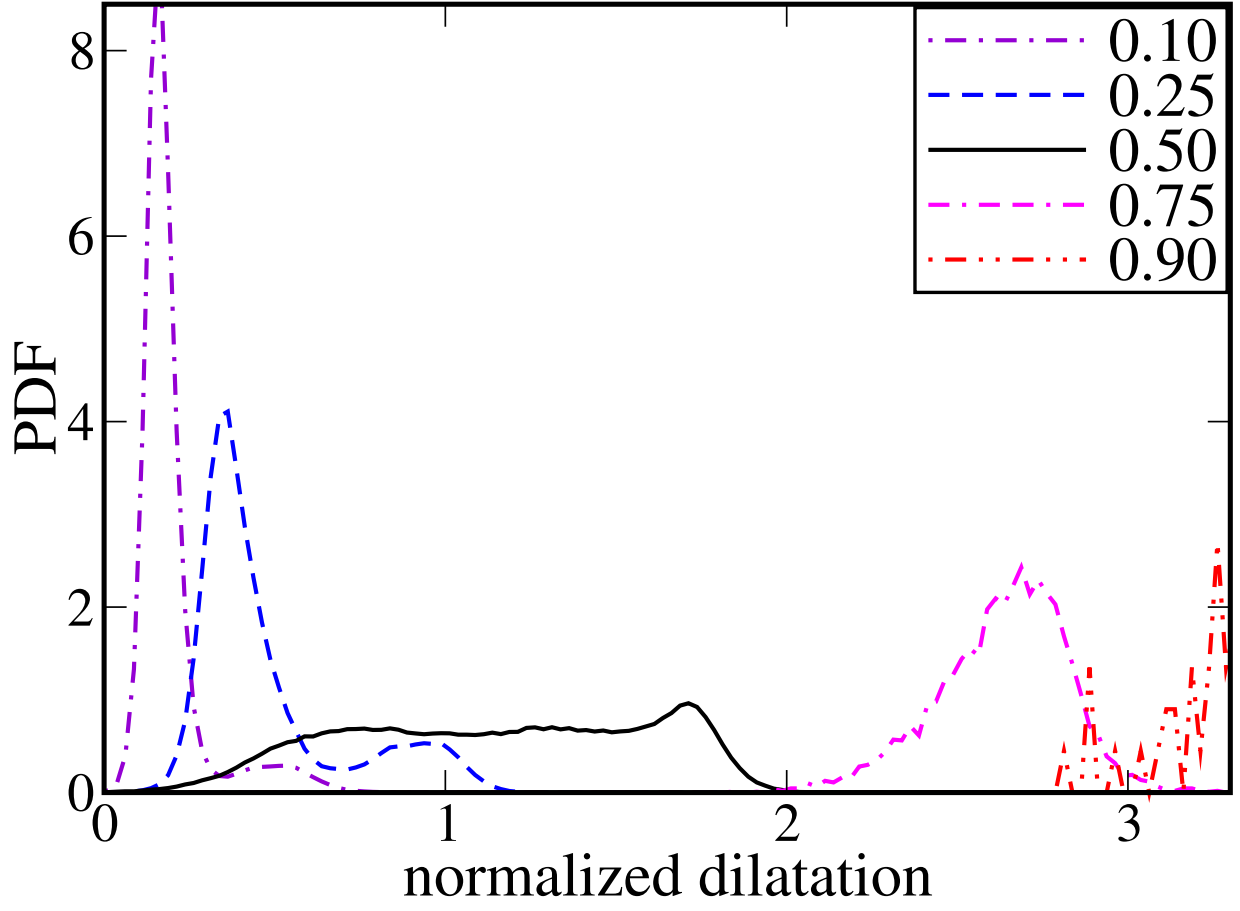
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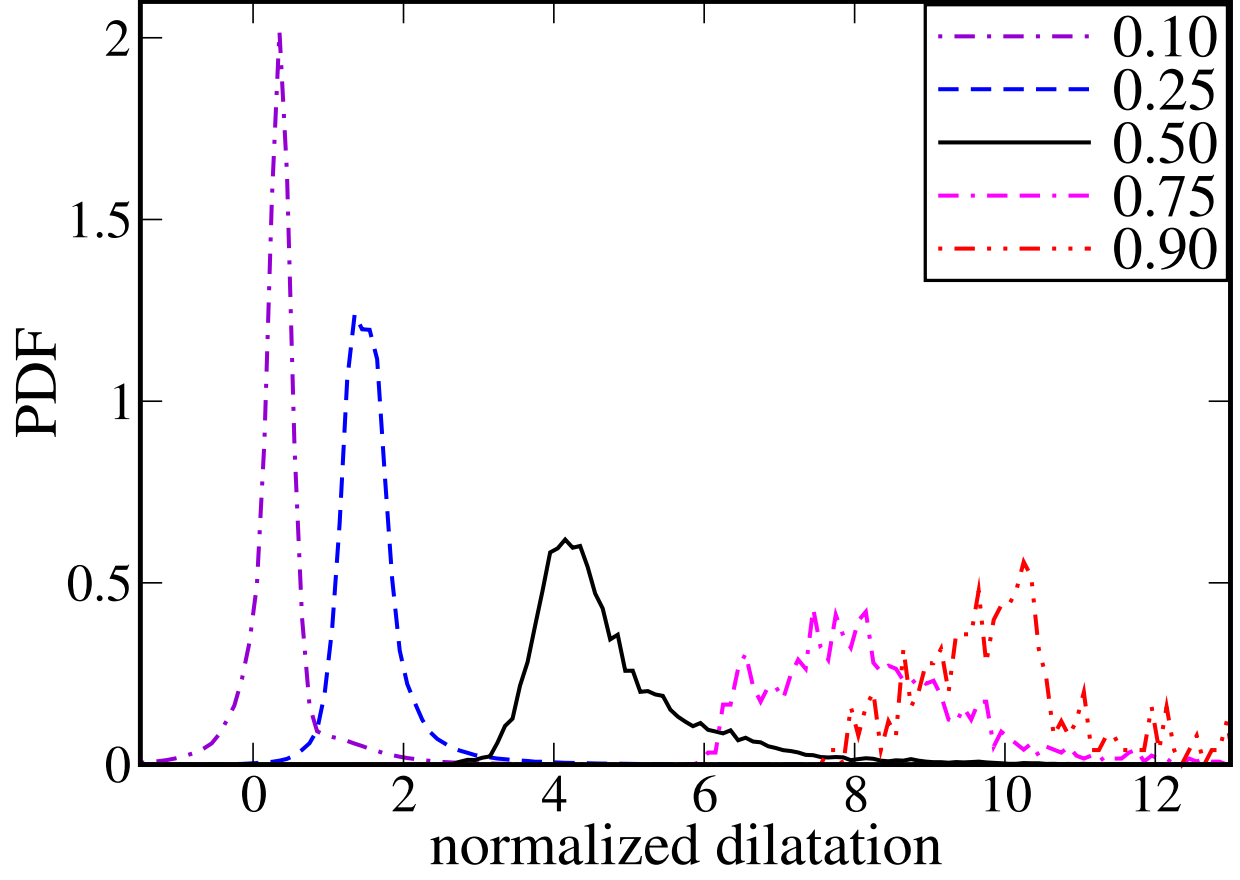
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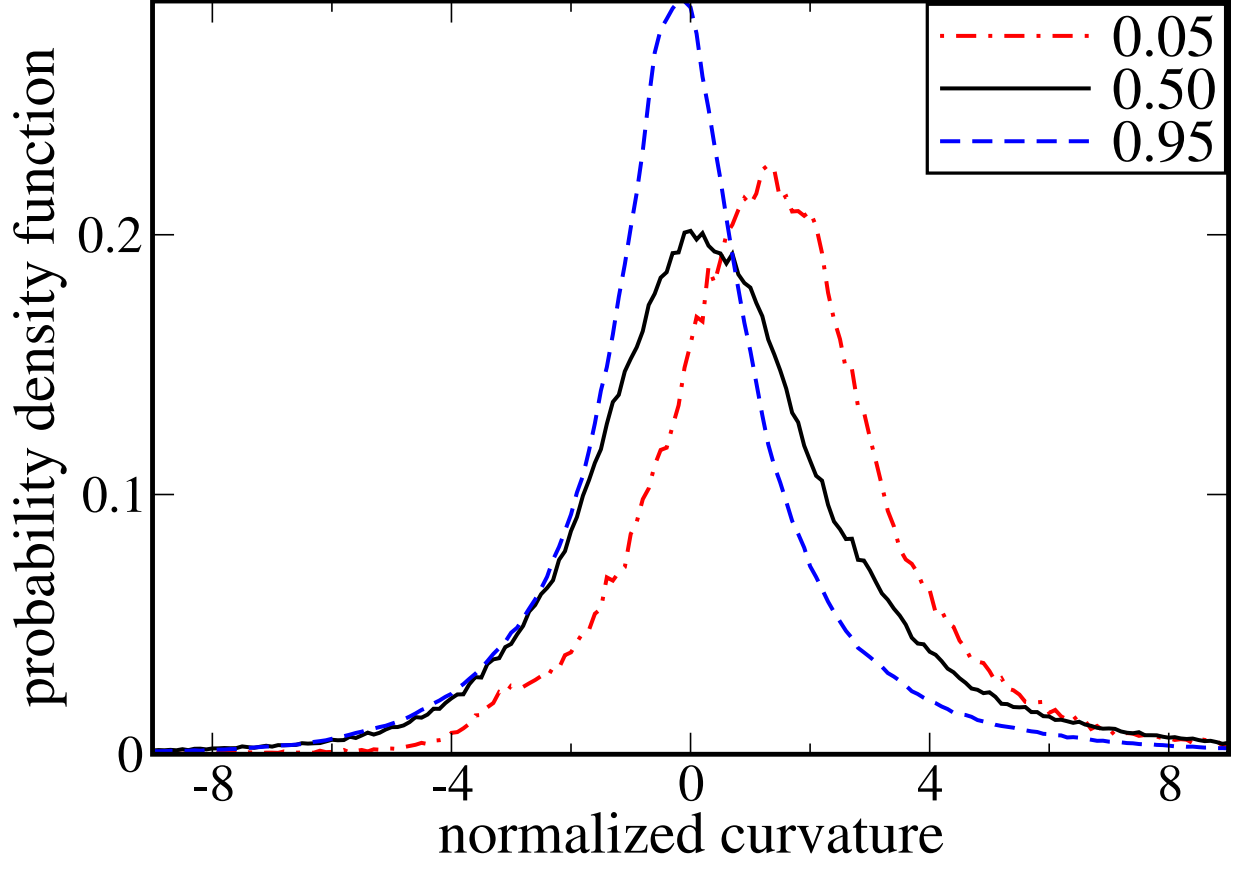
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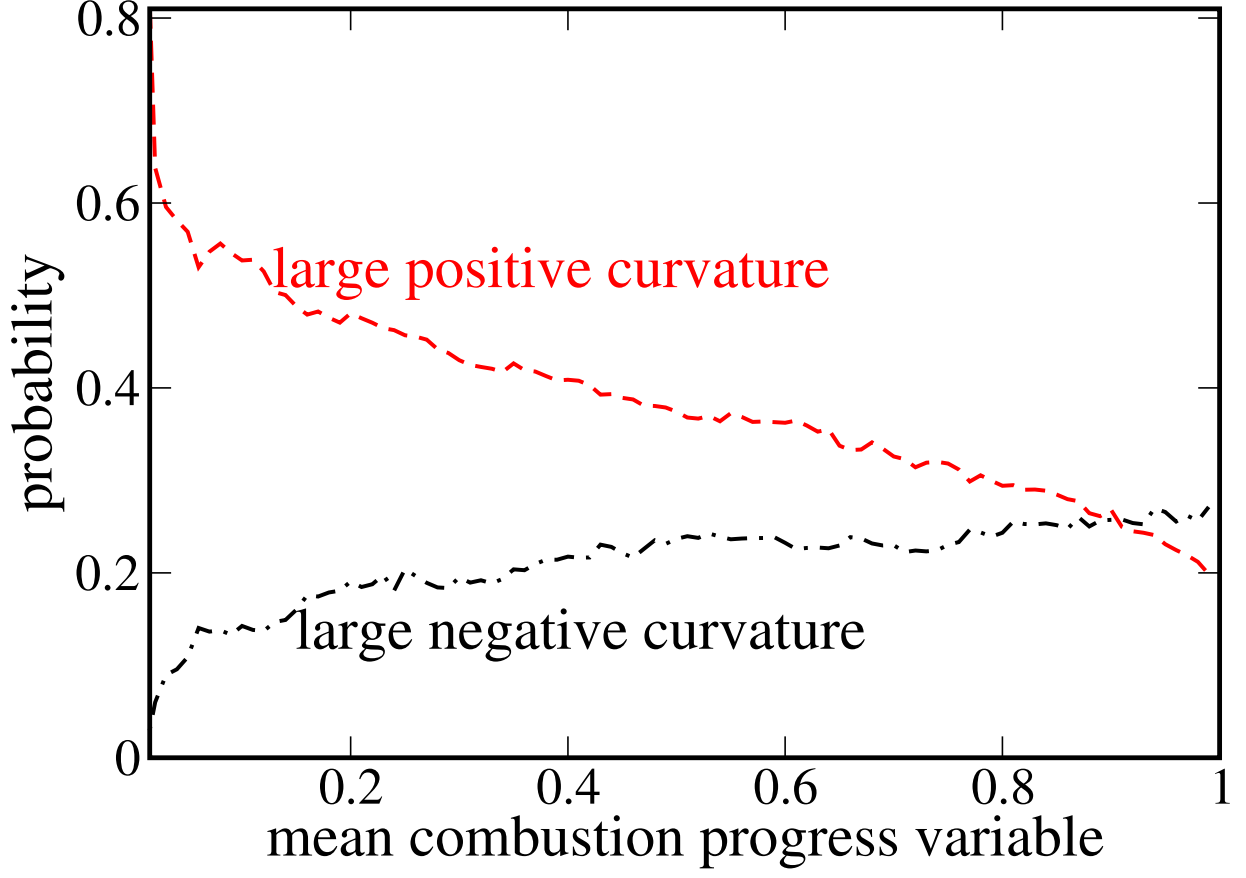
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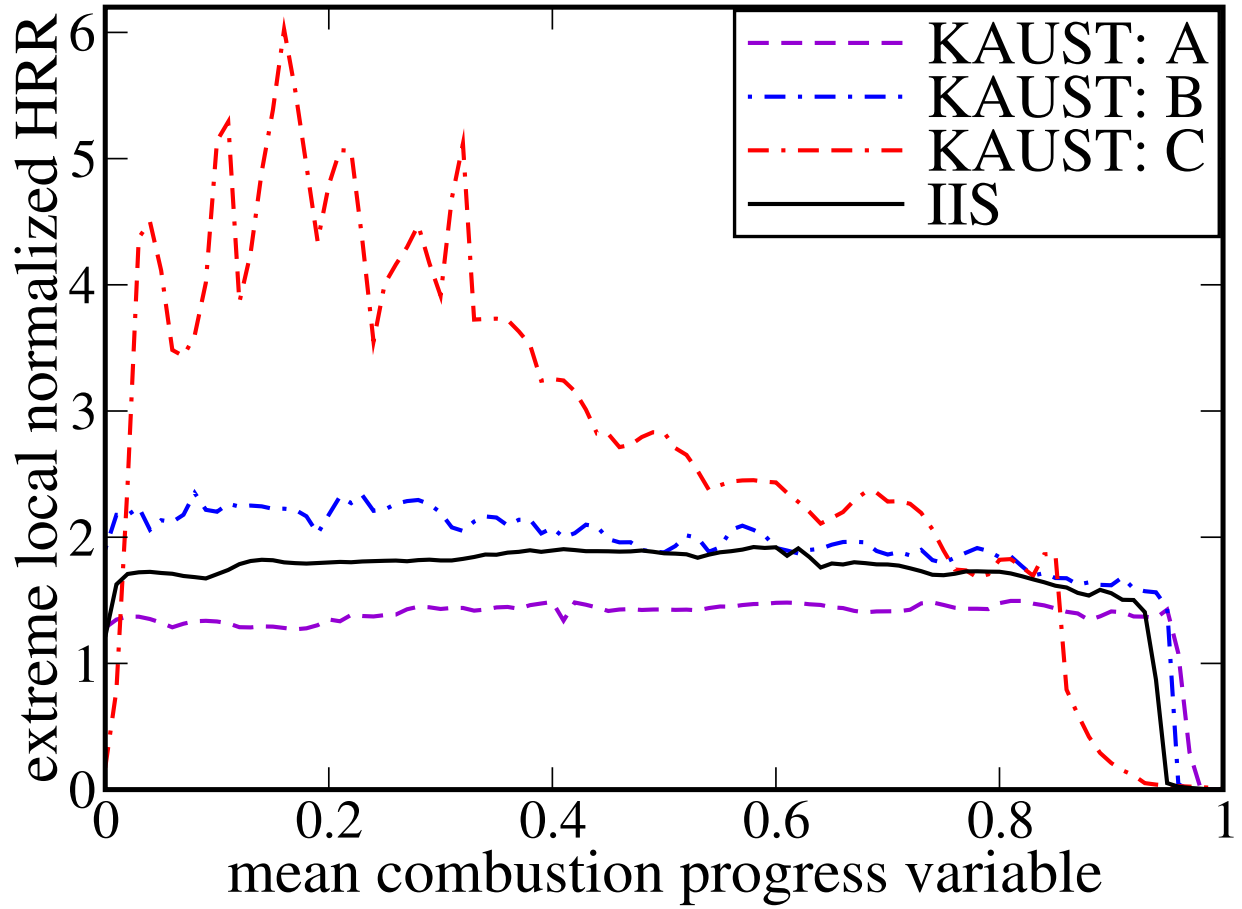


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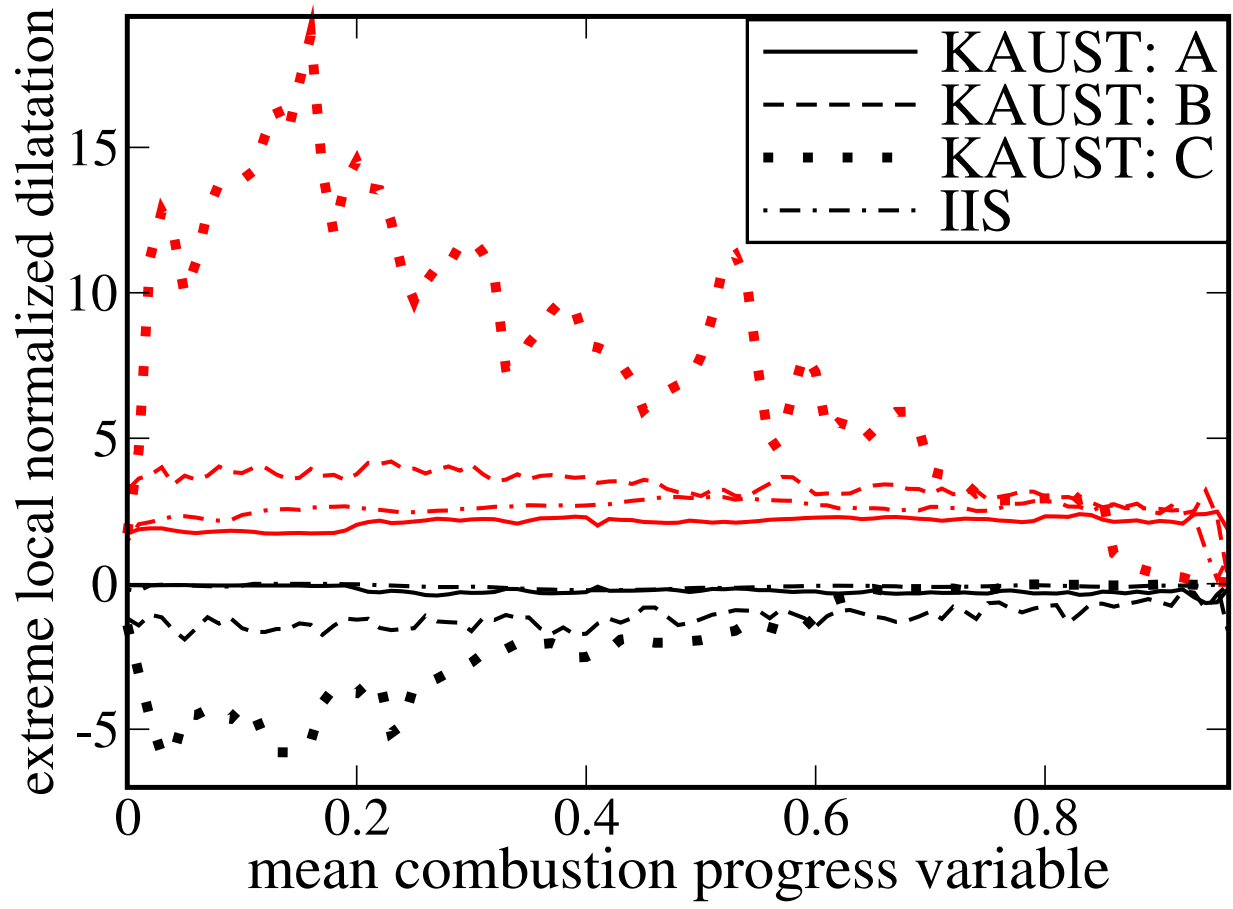
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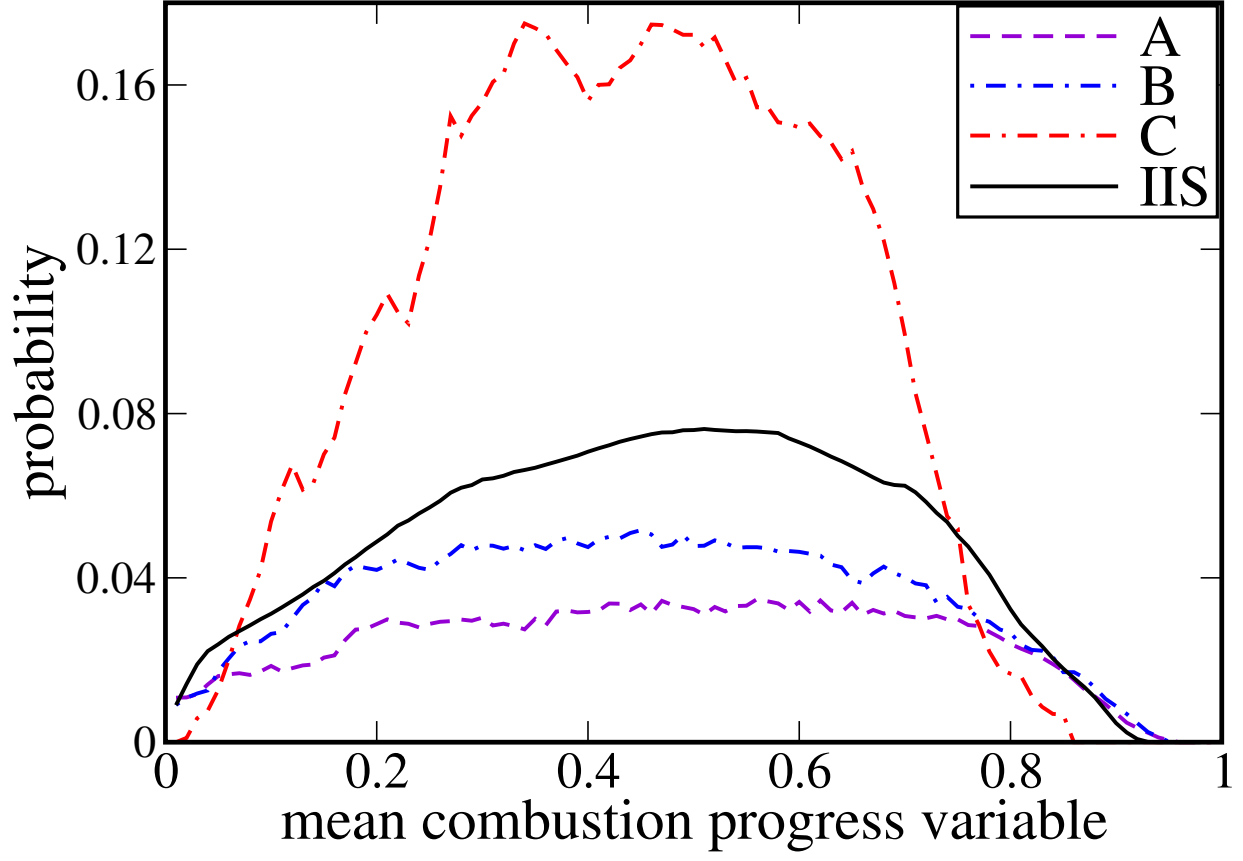


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